Supporting Information Part 2

DFT virtual screening identifies rhodium-amidinate complexes as potential homogeneous catalysts for methane to methanol oxidation

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Cartesian Coordinates

All numbers are in Ångströms.

Rh(NN) complexes

Table S4. $Rh^{I}(NN)(TFA)(TFAH)]^{-}$

Atom	x	y	z
Rh1	0.214562	0.061355	-0.01511
N2	-0.78223	-0.45637	1.738311
C3	3.146085	0.599577	0.807305
O4	3.759332	-0.18425	-0.00758
C5	-1.85404	-0.94608	1.096478
O6	1.965355	0.954555	0.824446
N7	-1.65999	-0.81572	-0.22295
C8	1.747419	-0.2098	-2.64304
O9	0.766498	0.297457	-2.06071
O10	2.819085	-0.69344	-2.18519
C11	1.591678	-0.30109	-4.18173
F12	2.761061	-0.51554	-4.81296
F13	0.768731	-1.33256	-4.50219
F14	1.051375	0.818441	-4.69923
C15	4.087713	1.16608	1.889824
F16	4.759778	0.180317	2.515118
F17	5.002489	1.992763	1.333277
F18	3.419439	1.86552	2.819558
H19	3.202787	-0.44152	-0.92459
C20	-5.32563	-2.63617	2.985291
C21	-4.71963	-3.29573	1.913724
C22	-3.59657	-2.74841	1.296321
C23	-3.05764	-1.53239	1.746003
C24	-3.67164	-0.87802	2.82593
C25	-4.79782	-1.42489	3.43764
H26	-6.20295	-3.06334	3.464774
H27	-5.12321	-4.24004	1.556799
H28	-3.12709	-3.25824	0.460787
H29	-3.25616	0.060574	3.179287
H30	-5.26387	-0.90435	4.270614
C31	0.592348	-1.05248	5.683478
C32	-0.22581	-2.01518	5.088781
C33	-0.69792	-1.85112	3.788312
C34	-0.37654	-0.69239	3.047024

C35	0.471285	0.26146	3.649471
C36	0.94358	0.081577	4.944922
H37	0.965326	-1.19273	6.694946
H38	-0.48852	-2.91835	5.636275
H39	-1.30074	-2.62957	3.334855
H40	0.763816	1.125717	3.064127
H41	1.601788	0.832077	5.377045
C42	-4.396	-1.07018	-3.42553
C43	-4.84315	-0.64892	-2.17175
C44	-3.96432	-0.54927	-1.09505
C45	-2.60345	-0.89345	-1.24431
C46	-2.15686	-1.28684	-2.52239
C47	-3.04221	-1.37759	-3.59078
H48	-5.08577	-1.13969	-4.26301
H49	-5.88766	-0.37871	-2.02927
H50	-4.32483	-0.19027	-0.1376
H51	-1.10261	-1.49669	-2.65692
H52	-2.66569	-1.68398	-4.56412

Table S5. $Rh^{I}(NN)(TFAH)_2$

Atom	x	y	z
Rh1	0.20678	0.083774	-0.14522
N2	-0.77554	-0.30277	1.612725
C3	3.116549	1.069604	0.025589
O4	3.41547	0.755905	-1.21672
C5	-1.81347	-0.89779	1.012892
O6	2.024374	0.977958	0.56988
N7	-1.62694	-0.82472	-0.31218
C8	0.228648	1.280276	-2.7733
O9	0.901684	0.384513	-2.23244
O10	-0.68409	1.962199	-2.17028
C11	0.428851	1.624982	-4.25852
F12	0.470848	2.952621	-4.42829
F13	1.57241	1.09498	-4.70587
F14	-0.5899	1.127105	-4.9722
C15	4.339134	1.602633	0.793877
F16	4.828763	2.689169	0.172981
F17	4.002228	1.931712	2.039912
F18	5.299146	0.665434	0.832481
H19	2.604526	0.461885	-1.69528

C20	-5.1319	-2.72729	3.014515
C21	-4.52122	-3.37605	1.939216
C22	-3.44684	-2.78106	1.281172
C23	-2.96607	-1.53212	1.701971
C24	-3.58018	-0.88734	2.78604
C25	-4.6609	-1.48151	3.434214
H26	-5.97186	-3.19144	3.524127
H27	-4.88286	-4.34662	1.611477
H28	-2.97374	-3.28256	0.442828
H29	-3.20821	0.077875	3.114938
H30	-5.13413	-0.97276	4.269317
C31	0.641625	-0.63141	5.566815
C32	0.052066	-1.73859	4.953761
C33	-0.42221	-1.65822	3.646014
C34	-0.33037	-0.44865	2.933957
C35	0.27998	0.65743	3.55006
C36	0.758093	0.564417	4.85398
H37	1.01505	-0.70239	6.584484
H38	-0.02909	-2.67931	5.492219
H39	-0.85805	-2.53003	3.170066
H40	0.367927	1.581267	2.987046
H41	1.22288	1.431081	5.316681
C42	-4.31949	-1.35434	-3.51045
C43	-4.77688	-0.82103	-2.30349
C44	-3.90869	-0.63842	-1.22999
C45	-2.55531	-1.01001	-1.34174
C46	-2.09838	-1.53614	-2.56355
C47	-2.97338	-1.70539	-3.63387
H48	-5.00104	-1.48598	-4.34583
H49	-5.81879	-0.52941	-2.19848
H50	-4.27099	-0.199	-0.30702
H51	-1.05253	-1.81751	-2.64862
H52	-2.60174	-2.11787	-4.56831
H53	-0.68262	1.573002	-1.17827

Table S6. [Rh^{III}(NN)$(TFA)_3$($TFAH^{eq}$)]$^-$

Atom	x	y	z
Rh1	0.305761	0.241313	-0.11171
N2	-0.60073	-0.27317	1.655134
C3	3.296179	0.908672	-0.03688

O4	3.412448	1.072497	-1.30211
C5	-1.77691	-0.53413	1.07121
O6	2.291188	0.630113	0.62512
N7	-1.67644	-0.25985	-0.22113
C8	0.368057	1.367504	-2.93513
O9	1.046202	0.674095	-2.06558
O10	-0.78683	1.738089	-2.88407
C11	1.188975	1.651963	-4.22295
F12	1.071753	0.611972	-5.0822
F13	0.744791	2.749713	-4.85401
F14	2.505165	1.823423	-3.97745
C15	4.611272	1.08364	0.750656
F16	5.609899	1.534265	-0.02015
F17	4.429719	1.957248	1.757317
F18	4.98651	-0.09199	1.282991
H19	2.495256	0.930203	-1.75453
C20	-5.27226	-1.89038	3.144764
C21	-4.91264	-2.48224	1.932416
C22	-3.78213	-2.04337	1.245048
C23	-2.99569	-1.01157	1.775383
C24	-3.35899	-0.42124	2.994021
C25	-4.49477	-0.85744	3.672423
H26	-6.15618	-2.23303	3.676958
H27	-5.51402	-3.28754	1.519186
H28	-3.50276	-2.50044	0.301505
H29	-2.74814	0.379129	3.399475
H30	-4.77177	-0.39162	4.61439
C31	1.122697	-1.67448	5.225183
C32	0.227925	-2.48956	4.529507
C33	-0.35482	-2.05294	3.341545
C34	-0.0642	-0.77021	2.843914
C35	0.846647	0.042892	3.541485
C36	1.433394	-0.40946	4.71877
H37	1.58432	-2.02634	6.144191
H38	-0.00455	-3.48438	4.901903
H39	-1.02044	-2.70488	2.786433
H40	1.084673	1.019089	3.132902
H41	2.139282	0.229842	5.242985
C42	-4.60695	-0.41692	-3.22295
C43	-4.79435	0.412349	-2.11586

C44	-3.82384	0.487116	-1.11842
C45	-2.66126	-0.28882	-1.21782
C46	-2.46551	-1.11576	-2.33426
C47	-3.43735	-1.17482	-3.32935
H48	-5.36292	-0.46567	-4.00275
H49	-5.69451	1.016544	-2.033
H50	-3.94716	1.150085	-0.2682
H51	-1.55599	-1.70632	-2.39092
H52	-3.28198	-1.81792	-4.19189
O53	-0.28809	2.159933	0.343327
C54	0.369785	3.20165	-0.0234
O55	1.428307	3.310275	-0.62814
C56	-0.36235	4.488542	0.456239
F57	0.21121	5.601957	-0.03183
F58	-1.65991	4.50543	0.087413
F59	-0.32873	4.579226	1.809429
O60	0.579057	-1.77643	-0.47115
C61	1.664253	-2.28709	-0.93782
O62	2.774023	-1.80513	-1.10642
C63	1.410909	-3.77016	-1.33457
F64	2.504639	-4.34964	-1.85637
F65	1.027432	-4.51257	-0.27056
F66	0.425121	-3.86193	-2.26148

Table S7. $Rh^{III}(NN)(TFA)_2(TFAH^{ax})(TFAH^{eq})$

Atom	x	y	z
Rh1	0.04057	0.294356	-0.35517
N2	-0.74949	-0.01531	1.482221
C3	2.99586	1.053322	-0.50832
O4	3.303117	0.24792	-1.42312
C5	-1.9436	-0.39451	1.008802
O6	1.939808	1.107714	0.169305
N7	-1.9053	-0.31679	-0.32572
C8	0.880159	0.845399	-3.42975
O9	0.447281	0.158469	-2.49607
O10	1.183873	2.086871	-3.44154
C11	1.115328	0.107296	-4.7686
F12	1.293525	0.953255	-5.78484
F13	2.204336	-0.66913	-4.65246
F14	0.059919	-0.67804	-5.04089

C15	4.066161	2.12958	-0.19859
F16	4.265365	2.888624	-1.28943
F17	3.698463	2.926005	0.811867
F18	5.229907	1.541487	0.1272
H19	1.00635	2.585761	-2.52084
C20	-5.26896	-1.67767	3.358769
C21	-5.0356	-2.25055	2.106585
C22	-3.95498	-1.82949	1.336515
C23	-3.09443	-0.83343	1.823174
C24	-3.3284	-0.2633	3.083539
C25	-4.41638	-0.68388	3.844084
H26	-6.11505	-2.00579	3.955942
H27	-5.69551	-3.0263	1.72961
H28	-3.7674	-2.273	0.363923
H29	-2.66516	0.511216	3.454934
H30	-4.59922	-0.23519	4.815919
C31	1.366481	-1.20989	4.90637
C32	0.562802	-2.13609	4.237989
C33	-0.14435	-1.76215	3.097766
C34	-0.06703	-0.43818	2.635901
C35	0.74782	0.490708	3.300474
C36	1.460754	0.10068	4.430483
H37	1.924259	-1.51062	5.788547
H38	0.497956	-3.15987	4.595726
H39	-0.74494	-2.4857	2.556386
H40	0.811411	1.502865	2.914189
H41	2.091442	0.822137	4.941734
C42	-4.91688	0.577648	-3.11984
C43	-5.00223	1.094512	-1.82562
C44	-4.01372	0.814128	-0.88532
C45	-2.9353	-0.01671	-1.23193
C46	-2.84303	-0.52579	-2.53755
C47	-3.83017	-0.22631	-3.47243
H48	-5.68509	0.809524	-3.85174
H49	-5.83411	1.736112	-1.54885
H50	-4.06459	1.242336	0.109991
H51	-1.98917	-1.13915	-2.80632
H52	-3.74941	-0.62243	-4.48076
O53	-0.67984	2.205052	-0.148
C54	-0.11382	3.265961	-0.55387

O55	0.751643	3.431283	-1.43005
C56	-0.62291	4.521845	0.202067
F57	-0.03897	5.637949	-0.24071
F58	-1.95421	4.648542	0.050037
F59	-0.36168	4.397698	1.517633
O60	0.503151	-1.7503	-0.32211
C61	1.388411	-2.39385	-0.91739
O62	2.409414	-1.98976	-1.55287
C63	1.254328	-3.93616	-0.89576
F64	2.331848	-4.48027	-0.31031
F65	0.163509	-4.32244	-0.22498
F66	1.169937	-4.39785	-2.15312
H67	2.697785	-0.90946	-1.49947

Table S8. $Rh^{III}(NN)(TFA)_2(TFAH^{ax})_2$

Atom	x	y	z
Rh1	0.078247	0.228667	-0.41409
N2	-0.64414	-0.08765	1.466256
C3	3.077873	0.961704	-0.55911
O4	3.45311	0.045277	-1.32603
C5	-1.84982	-0.47615	1.032505
O6	1.957344	1.146094	-0.01667
N7	-1.83923	-0.45349	-0.30387
C8	1.060945	1.002586	-3.24467
O9	0.444597	0.1849	-2.51399
O10	1.400632	2.185562	-3.00724
C11	1.452392	0.430597	-4.6312
F12	2.122912	1.317956	-5.36974
F13	2.221885	-0.66083	-4.47032
F14	0.343459	0.067334	-5.30254
C15	4.118978	2.058022	-0.21736
F16	5.299697	1.82947	-0.79715
F17	3.66431	3.255657	-0.62869
F18	4.302199	2.114178	1.115448
H19	0.948268	2.85626	-1.9979
C20	-5.18881	-1.53552	3.474428
C21	-4.98517	-2.18317	2.254074
C22	-3.89813	-1.84083	1.454171
C23	-3.0011	-0.84937	1.879558
C24	-3.20575	-0.20368	3.108354

C25	-4.29976	-0.54552	3.898693
H26	-6.04029	-1.80172	4.094307
H27	-5.67389	-2.95542	1.924479
H28	-3.73561	-2.34231	0.505625
H29	-2.51397	0.567512	3.431576
H30	-4.45932	-0.03819	4.845533
C31	1.543717	-1.16536	4.887405
C32	0.647331	-2.07854	4.328517
C33	-0.08527	-1.7436	3.192271
C34	0.059023	-0.46872	2.620195
C35	0.967887	0.445332	3.175786
C36	1.705107	0.093245	4.302524
H37	2.120825	-1.43655	5.766626
H38	0.528818	-3.06484	4.768446
H39	-0.76042	-2.46268	2.740317
H40	1.089745	1.416255	2.706993
H41	2.408632	0.804598	4.725364
C42	-4.89049	0.225084	-3.10694
C43	-4.89102	0.937944	-1.906
C44	-3.89001	0.727073	-0.96025
C45	-2.88898	-0.22577	-1.2085
C46	-2.88354	-0.93668	-2.41841
C47	-3.8818	-0.70799	-3.36107
H48	-5.66713	0.402431	-3.8453
H49	-5.66515	1.674633	-1.7102
H50	-3.8658	1.303205	-0.041
H51	-2.09277	-1.65826	-2.59831
H52	-3.87229	-1.25903	-4.29704
O53	-0.76078	2.11761	-0.17098
C54	-0.3573	3.261761	-0.46857
O55	0.528028	3.627661	-1.29267
C56	-1.05122	4.400775	0.317464
F57	-0.66262	4.340907	1.603973
F58	-0.7432	5.604241	-0.16712
F59	-2.38436	4.244516	0.271207
O60	0.557951	-1.79824	-0.43412
C61	1.344874	-2.44725	-1.15422
O62	2.389135	-2.0744	-1.76262
C63	0.95828	-3.93307	-1.34705
F64	1.937816	-4.63811	-1.91385

F65	0.649159	-4.49059	-0.16708
F66	-0.12922	-3.99122	-2.141
H67	2.762789	-1.04223	-1.55926

Table S9. $Rh^{III}(NN)(TFA)_2(TFAH^{eq})_2$

Atom	x	y	z
Rh1	0.10482	0.156298	-0.32844
N2	-0.69549	-0.15043	1.499172
C3	3.076495	1.134379	-0.48888
O4	3.501779	0.363986	-1.42113
C5	-1.89033	-0.49709	1.02755
O6	2.043591	1.021132	0.182838
N7	-1.82976	-0.4559	-0.31514
C8	0.651978	0.799802	-3.45716
O9	0.504378	0.065307	-2.47465
O10	0.806079	2.070409	-3.49784
C11	0.609774	0.120295	-4.8473
F12	1.207115	0.862077	-5.78269
F13	1.203847	-1.07676	-4.79649
F14	-0.67999	-0.05811	-5.198
C15	4.0163	2.328769	-0.20449
F16	4.276639	2.987131	-1.34203
F17	3.464402	3.173475	0.669772
F18	5.174948	1.877743	0.305829
H19	0.799067	2.538594	-2.54427
C20	-5.35162	-1.56605	3.283513
C21	-5.10523	-2.17209	2.049873
C22	-3.97472	-1.82568	1.315393
C23	-3.07804	-0.87093	1.81929
C24	-3.32445	-0.26815	3.062155
C25	-4.46188	-0.61478	3.786862
H26	-6.23732	-1.83452	3.852201
H27	-5.79449	-2.9146	1.658983
H28	-3.77661	-2.29429	0.356844
H29	-2.63468	0.47617	3.44676
H30	-4.65509	-0.13986	4.744098
C31	1.285059	-0.99782	5.09788
C32	0.550805	-2.00229	4.463992
C33	-0.11134	-1.74179	3.266555
C34	-0.05626	-0.45366	2.712324

C35	0.686234	0.556022	3.342789
C36	1.354215	0.277867	4.532028
H37	1.808072	-1.21078	6.02561
H38	0.50542	-2.99886	4.893826
H39	-0.65845	-2.52394	2.750323
H40	0.722136	1.541834	2.889388
H41	1.928522	1.060022	5.01984
C42	-4.71278	0.699254	-3.14737
C43	-4.7479	1.254039	-1.86625
C44	-3.80263	0.887083	-0.91119
C45	-2.82474	-0.0702	-1.22932
C46	-2.78748	-0.62354	-2.51917
C47	-3.72561	-0.23469	-3.47121
H48	-5.44377	1.00102	-3.8919
H49	-5.50338	1.992655	-1.61326
H50	-3.80683	1.345227	0.072129
H51	-2.0155	-1.34783	-2.75714
H52	-3.684	-0.66134	-4.46913
O53	-0.60887	2.093865	-0.07515
C54	-0.03379	3.155231	-0.45701
O55	0.777066	3.33416	-1.38567
C56	-0.427	4.384373	0.402712
F57	0.155052	5.505046	-0.03052
F58	-1.76089	4.561245	0.382244
F59	-0.0527	4.178947	1.68271
O60	0.577249	-1.84961	-0.32695
C61	1.548687	-2.3917	-0.93544
O62	2.538808	-1.88855	-1.49345
C63	1.424349	-3.93804	-0.96903
F64	2.482245	-4.50937	-1.55098
F65	1.310616	-4.42643	0.279985
F66	0.320661	-4.289	-1.65721
H67	2.97654	-0.56826	-1.46571

Table S10. $[Rh^{III}(NN)(TFA)_2(TFAH^{eq})(CH_3{}^{ax})]^-$

Atom	x	y	z
Rh1	0.449372	0.117393	0.025687
N2	-0.56406	-0.30594	1.816716
C3	3.250502	1.383233	0.588577
O4	2.990716	2.527943	1.091875

C5	-1.73742	-0.43318	1.195671
O6	2.542564	0.374565	0.487674
N7	-1.55277	-0.29105	-0.12151
C8	1.730021	1.202877	-2.47079
O9	0.889911	0.359741	-1.99516
O10	2.503271	1.982967	-1.92298
C11	1.686944	1.191371	-4.0269
F12	2.690133	1.909343	-4.56627
F13	1.780628	-0.06341	-4.52726
F14	0.525584	1.717005	-4.4831
C15	4.734379	1.233046	0.182094
F16	5.255759	2.377521	-0.27625
F17	5.451006	0.865189	1.276998
F18	4.901151	0.285228	-0.7467
H19	1.966512	2.700203	1.44998
C20	-5.48694	-1.25773	3.109235
C21	-5.11948	-1.95441	1.956433
C22	-3.9069	-1.67759	1.328327
C23	-3.04468	-0.70534	1.853988
C24	-3.41932	-0.00564	3.009711
C25	-4.63644	-0.28059	3.630446
H26	-6.43389	-1.47347	3.597815
H27	-5.77854	-2.7142	1.544568
H28	-3.61803	-2.21336	0.429408
H29	-2.76209	0.762034	3.40307
H30	-4.92147	0.270965	4.522511
C31	0.575102	-1.46734	5.701599
C32	-0.32302	-2.2562	4.98121
C33	-0.71634	-1.89257	3.694711
C34	-0.22212	-0.71119	3.109099
C35	0.691097	0.074487	3.835408
C36	1.080812	-0.30303	5.11711
H37	0.883081	-1.75926	6.702242
H38	-0.7136	-3.17268	5.41762
H39	-1.39553	-2.52485	3.133025
H40	1.064045	0.987638	3.382245
H41	1.78242	0.321327	5.665011
C42	-4.31212	0.800467	-3.10305
C43	-4.45004	1.319661	-1.81478
C44	-3.53952	0.987091	-0.81423

C45	-2.48749	0.096445	-1.08907
C46	-2.33076	-0.39734	-2.39493
C47	-3.23932	-0.04776	-3.38928
H48	-5.02004	1.071833	-3.88208
H49	-5.26033	2.008804	-1.58883
H50	-3.61521	1.43594	0.16957
H51	-1.47931	-1.03423	-2.60895
H52	-3.10428	-0.43519	-4.396
O53	-0.36997	2.321971	0.23405
C54	-0.20552	3.015765	1.249656
O55	0.812848	3.142975	1.990667
C56	-1.45332	3.825029	1.69617
F57	-1.21301	4.659394	2.72191
F58	-1.95414	4.556034	0.682913
F59	-2.43589	2.970959	2.098625
C60	0.908001	-1.85905	-0.1548
H61	1.72918	-2.07565	0.534264
H62	0.03735	-2.47796	0.082317
H63	1.220932	-2.01781	-1.19016

Table S11. $[Rh^{III}(NN)(TFA)_2(TFAH^{ax})(CH_3{}^{ax})]^-$

Atom	x	y	z
Rh1	0.425092	0.113142	-0.38675
N2	-0.41291	-0.24181	1.497843
C3	3.155789	1.325677	0.42915
O4	2.777101	2.355919	1.036578
C5	-1.64732	-0.40543	1.000349
O6	2.515247	0.393041	-0.10464
N7	-1.60466	-0.30197	-0.32723
C8	0.792232	-0.06667	-3.4173
O9	0.912833	0.614742	-2.34506
O10	0.32091	-1.18407	-3.62861
C11	1.361023	0.67282	-4.66395
F12	0.421856	0.754729	-5.63543
F13	1.791218	1.924475	-4.4203
F14	2.406511	-0.01729	-5.17981
C15	4.699782	1.192349	0.34043
F16	5.218517	2.211671	-0.37725
F17	5.248464	1.245631	1.575053
F18	5.098363	0.04585	-0.23023

H19	1.478444	2.880844	1.276216
C20	-5.18834	-1.05002	3.334845
C21	-4.92897	-1.85463	2.223503
C22	-3.78212	-1.64546	1.459884
C23	-2.87784	-0.63291	1.808928
C24	-3.14226	0.172477	2.925815
C25	-4.29506	-0.03451	3.681035
H26	-6.08586	-1.21129	3.926613
H27	-5.62304	-2.64423	1.947938
H28	-3.58074	-2.26186	0.589109
H29	-2.45334	0.970707	3.182766
H30	-4.49648	0.60048	4.539684
C31	1.16881	-1.41242	5.228102
C32	0.131535	-2.15007	4.656158
C33	-0.40541	-1.7859	3.422882
C34	0.077149	-0.65155	2.74104
C35	1.134074	0.077438	3.316896
C36	1.668923	-0.30122	4.544282
H37	1.589027	-1.70474	6.18686
H38	-0.25747	-3.02886	5.16556
H39	-1.19305	-2.38375	2.97763
H40	1.521809	0.942646	2.790555
H41	2.48323	0.280187	4.969559
C42	-4.75639	0.384726	-3.0366
C43	-4.77805	1.001506	-1.78472
C44	-3.73982	0.799865	-0.87737
C45	-2.66993	-0.05061	-1.20724
C46	-2.6332	-0.64504	-2.47935
C47	-3.67249	-0.42724	-3.38002
H48	-5.56432	0.552202	-3.7446
H49	-5.59888	1.662339	-1.51565
H50	-3.74057	1.318535	0.073829
H51	-1.76792	-1.24003	-2.7559
H52	-3.62727	-0.89096	-4.36226
O53	-0.50333	2.411686	-0.12777
C54	-0.41867	3.145234	0.843438
O55	0.610176	3.394937	1.592678
C56	-1.66514	3.912554	1.34535
F57	-1.44456	5.240525	1.385798
F58	-2.72932	3.69094	0.56275

F59	-1.98363	3.511556	2.598934
C60	0.86763	-1.87186	-0.51506
H61	1.870555	-1.99433	-0.09931
H62	0.137723	-2.44899	0.059772
H63	0.827388	-2.13113	-1.57266

Table S12. $Rh^{III}(NN)(TFA)(TFAH^{eq})_2(CH_3^{ax})$

Atom	x	y	z
Rh1	0.290833	0.044456	-0.24426
N2	-0.55491	-0.49302	1.520254
C3	3.340715	1.152492	0.630463
O4	3.385225	2.45126	0.617863
C5	-1.7621	-0.67841	1.001045
O6	2.42747	0.410935	0.294335
N7	-1.65795	-0.52848	-0.33508
C8	0.908106	1.383457	-3.06779
O9	0.709392	0.404221	-2.35018
O10	1.134676	2.611582	-2.74406
C11	0.913513	1.184984	-4.60155
F12	0.009003	1.994117	-5.17335
F13	2.127393	1.483517	-5.09407
F14	0.620709	-0.07853	-4.92035
C15	4.657504	0.542148	1.164625
F16	4.838849	0.910513	2.44347
F17	4.619196	-0.79003	1.101427
F18	5.699563	0.981027	0.441378
H19	1.149383	2.827487	-1.72669
C20	-5.35543	-1.66036	3.102765
C21	-5.07498	-2.25947	1.87307
C22	-3.90606	-1.93584	1.188852
C23	-3.00235	-1.01313	1.737402
C24	-3.28614	-0.41636	2.974988
C25	-4.46168	-0.73783	3.64976
H26	-6.2697	-1.9113	3.633304
H27	-5.76777	-2.97855	1.445681
H28	-3.68567	-2.39678	0.231089
H29	-2.59322	0.303189	3.398185
H30	-4.68019	-0.26648	4.603536
C31	0.96187	-1.1865	5.379827
C32	0.276525	-2.20198	4.710783

C33	-0.23267	-1.9875	3.431266
C34	-0.07268	-0.73732	2.815332
C35	0.616623	0.283708	3.488108
C36	1.130336	0.05508	4.762464
H37	1.363657	-1.36139	6.373639
H38	0.14588	-3.17254	5.181487
H39	-0.75068	-2.78075	2.901699
H40	0.717483	1.256175	3.015993
H41	1.657351	0.853247	5.277915
C42	-4.51279	0.806531	-3.12698
C43	-4.57188	1.268358	-1.81074
C44	-3.6349	0.846865	-0.8697
C45	-2.63692	-0.07219	-1.23639
C46	-2.5719	-0.52446	-2.56462
C47	-3.50424	-0.08487	-3.50062
H48	-5.24042	1.146515	-3.85827
H49	-5.34245	1.97561	-1.51608
H50	-3.66193	1.23401	0.143014
H51	-1.78366	-1.21668	-2.84341
H52	-3.44484	-0.44233	-4.52488
O53	-0.56852	2.192529	0.296268
C54	0.161356	3.18584	0.341683
O55	1.215861	3.409214	-0.35643
C56	-0.15086	4.25663	1.415238
F57	0.136602	5.495982	0.998762
F58	-1.43173	4.221767	1.80003
F59	0.621322	3.988383	2.500146
C60	0.874909	-1.88676	-0.54357
H61	1.802088	-2.02863	0.016547
H62	0.101194	-2.57547	-0.19892
H63	1.042591	-2.00505	-1.61728
H64	2.528606	2.862885	0.253882

Table S13. $Rh^{III}(NN)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.333942	0.182419	-0.29363
N2	-0.44348	-0.40358	1.498032
C3	3.436108	0.529414	-0.11026
O4	3.720332	-0.13513	-1.11503
C5	-1.67114	-0.60752	1.003565

O6	2.285426	0.909319	0.290633
N7	-1.62147	-0.41109	-0.31987
C8	1.277927	0.387253	-3.30573
O9	0.545107	0.733392	-2.37715
O10	2.443322	-0.16016	-3.2597
C11	0.732675	0.573378	-4.74059
F12	1.707454	0.562807	-5.65427
F13	-0.11571	-0.44118	-5.00875
F14	0.06094	1.724891	-4.83686
C15	4.588974	0.947249	0.836291
F16	5.785151	0.795083	0.265982
F17	4.44848	2.241548	1.193961
F18	4.547286	0.20096	1.955786
H19	1.884544	2.343072	0.945722
C20	-5.16238	-1.61767	3.261753
C21	-4.94602	-2.20249	2.012416
C22	-3.81146	-1.8751	1.273688
C23	-2.87697	-0.9638	1.787728
C24	-3.09564	-0.38341	3.046276
C25	-4.2372	-0.70689	3.775548
H26	-6.05068	-1.87077	3.833667
H27	-5.6629	-2.91311	1.611536
H28	-3.64336	-2.32482	0.300195
H29	-2.37415	0.322866	3.444293
H30	-4.40431	-0.24771	4.745557
C31	1.324478	-1.80315	5.054594
C32	0.388965	-2.59601	4.387987
C33	-0.20138	-2.15408	3.205889
C34	0.12441	-0.88947	2.686377
C35	1.074608	-0.09974	3.353789
C36	1.668407	-0.55681	4.526965
H37	1.787566	-2.15639	5.971263
H38	0.124556	-3.57368	4.781654
H39	-0.91175	-2.78385	2.681008
H40	1.33635	0.87006	2.945235
H41	2.40122	0.066202	5.032025
C42	-4.62793	0.684373	-3.05542
C43	-4.68949	1.154091	-1.74233
C44	-3.7048	0.808199	-0.81937
C45	-2.65264	-0.04004	-1.20178

C46	-2.5864	-0.49978	-2.52625
C47	-3.56779	-0.13752	-3.44419
H48	-5.39287	0.966538	-3.77301
H49	-5.50044	1.809077	-1.43575
H50	-3.73978	1.199592	0.191592
H51	-1.75703	-1.13319	-2.82247
H52	-3.501	-0.49697	-4.46719
O53	-0.39166	2.414028	0.166033
C54	0.213547	3.256427	0.808296
O55	1.44718	3.197346	1.244954
C56	-0.46179	4.587935	1.206644
F57	0.178658	5.618129	0.630263
F58	-1.73843	4.603399	0.819073
F59	-0.4138	4.74753	2.540028
C60	0.916235	-1.75406	-0.58522
H61	1.82431	-1.92751	-0.00256
H62	0.12412	-2.42793	-0.25334
H63	1.113678	-1.9174	-1.64828
H64	2.860839	-0.20732	-2.30432

Table S14. $[Rh^{IV}(NN)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax})]^+$

Atom	x	y	z
Rh1	0.35159	0.14973	-0.26946
N2	-0.42007	-0.54722	1.49285
C3	3.441495	0.442941	-0.1423
O4	3.702866	-0.20264	-1.15927
C5	-1.69488	-0.6274	1.028811
O6	2.288508	0.828893	0.277614
N7	-1.62524	-0.33603	-0.28025
C8	1.277264	0.598856	-3.24816
O9	0.552063	0.835386	-2.27
O10	2.422673	0.025915	-3.28457
C11	0.71203	0.982604	-4.63763
F12	1.669303	1.080587	-5.55274
F13	-0.15064	0.008615	-5.00653
F14	0.044989	2.135134	-4.55959
C15	4.595134	0.856451	0.807252
F16	5.785274	0.574584	0.297382
F17	4.517913	2.17791	1.055522
F18	4.453477	0.202593	1.981533

H19	1.952273	2.423315	0.803716
C20	-5.20704	-1.4791	3.298477
C21	-4.88752	-2.27029	2.192453
C22	-3.74566	-1.99589	1.442508
C23	-2.91064	-0.92983	1.81259
C24	-3.22999	-0.13867	2.92812
C25	-4.38122	-0.41283	3.662746
H26	-6.10062	-1.69326	3.876897
H27	-5.52806	-3.10092	1.912982
H28	-3.49853	-2.60876	0.580527
H29	-2.58535	0.688414	3.211241
H30	-4.63298	0.204854	4.519203
C31	1.360425	-1.8971	5.031157
C32	0.109947	-2.41069	4.656621
C33	-0.51508	-1.97655	3.499864
C34	0.118737	-1.00286	2.681255
C35	1.3933	-0.51057	3.055047
C36	1.998527	-0.95022	4.221222
H37	1.8374	-2.2443	5.942537
H38	-0.37188	-3.16423	5.271612
H39	-1.46713	-2.40053	3.210944
H40	1.889636	0.206561	2.415682
H41	2.973436	-0.56126	4.49644
C42	-4.55505	0.396092	-3.17349
C43	-4.83782	0.683226	-1.83122
C44	-3.89734	0.434429	-0.84316
C45	-2.63924	-0.10376	-1.20264
C46	-2.35219	-0.37039	-2.55842
C47	-3.30953	-0.13064	-3.5322
H48	-5.30093	0.593889	-3.93709
H49	-5.7955	1.11566	-1.5594
H50	-4.11058	0.685309	0.18798
H51	-1.38378	-0.77249	-2.8238
H52	-3.08173	-0.34368	-4.57136
O53	-0.38578	2.327633	0.291723
C54	0.248565	3.262325	0.765283
O55	1.526442	3.292715	1.034545
C56	-0.47423	4.566609	1.175128
F57	0.292486	5.634895	0.957835
F58	-1.61316	4.691044	0.492236

F59	-0.76013	4.489423	2.487911
C60	0.920135	-1.77895	-0.67935
H61	1.812611	-1.99306	-0.08859
H62	0.113814	-2.46386	-0.4108
H63	1.140453	-1.85916	-1.74528
H64	2.860009	-0.14781	-2.35326

Table S15. $Rh^{IV}(NN)(TFA)_2(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.45876	0.214597	-0.26317
N2	-0.28923	-0.46187	1.494311
C3	3.542474	0.381993	-0.22324
O4	3.806586	-0.07372	-1.35774
C5	-1.57369	-0.52427	1.046917
O6	2.433273	0.658241	0.302183
N7	-1.51995	-0.22291	-0.24944
C8	1.270228	0.597586	-3.28541
O9	0.558477	0.828098	-2.29675
O10	2.439204	0.093982	-3.34597
C11	0.630943	0.908317	-4.66002
F12	1.544348	1.017066	-5.62701
F13	-0.20471	-0.11018	-4.97689
F14	-0.08438	2.034798	-4.60742
C15	4.766958	0.698941	0.674929
F16	5.801425	-0.10064	0.389288
F17	5.147026	1.974115	0.481073
F18	4.470856	0.5457	1.98128
C20	-5.04279	-1.56515	3.309615
C21	-4.67684	-2.32928	2.199889
C22	-3.5515	-1.98092	1.45485
C23	-2.78499	-0.86692	1.828192
C24	-3.15497	-0.09413	2.939216
C25	-4.28576	-0.4487	3.672353
H26	-5.92101	-1.83706	3.888525
H27	-5.26616	-3.19542	1.913594
H28	-3.26253	-2.57326	0.591201
H29	-2.57589	0.789239	3.183749
H30	-4.57929	0.15336	4.527315
C31	1.451514	-1.61468	5.119024
C32	0.246035	-2.20664	4.721233

C33	-0.36176	-1.84008	3.530573
C34	0.243948	-0.85822	2.706329
C35	1.473824	-0.28309	3.101094
C36	2.060771	-0.65783	4.301601
H37	1.916015	-1.90805	6.055912
H38	-0.21705	-2.96684	5.343331
H39	-1.27931	-2.32224	3.221126
H40	1.944781	0.446105	2.454713
H41	3.001626	-0.20396	4.596642
C42	-4.56982	0.69873	-2.96089
C43	-4.69577	1.098163	-1.62642
C44	-3.70393	0.795515	-0.70113
C45	-2.56781	0.077872	-1.12239
C46	-2.42502	-0.29543	-2.4702
C47	-3.43022	0.006613	-3.38015
H48	-5.3501	0.943505	-3.67566
H49	-5.5648	1.666572	-1.30877
H50	-3.7649	1.151982	0.319729
H51	-1.52896	-0.81638	-2.78329
H52	-3.31648	-0.28583	-4.4194
O53	0.08905	2.34679	0.131207
C54	-0.75859	2.801797	0.963016
O55	-1.58701	2.202919	1.661561
C56	-0.68989	4.35092	1.082643
F57	-1.61993	4.832637	1.92527
F58	0.518887	4.740666	1.542256
F59	-0.88204	4.938169	-0.1172
C60	0.955798	-1.75292	-0.69178
H61	1.824143	-2.02393	-0.08564
H62	0.121027	-2.41763	-0.45367
H63	1.205386	-1.84107	-1.7521
H64	2.959449	-0.02306	-2.38302

Table S16. $Rh^{IV}(NN)(TFA)_2(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.393419	0.157626	-0.19691
N2	-0.36008	-0.64261	1.552571
C3	3.122923	1.414886	0.00719
O4	2.837144	2.516308	-0.48024
C5	-1.64151	-0.63335	1.124464

O6	2.391211	0.407622	0.269752
N7	-1.62328	-0.23424	-0.15994
C8	1.480192	0.856865	-2.92629
O9	0.536281	1.006728	-2.04656
O10	2.506754	0.205938	-2.87495
C11	1.111382	1.641619	-4.21601
F12	2.072452	1.559505	-5.14142
F13	-0.02741	1.130975	-4.75654
F14	0.886283	2.943629	-3.95639
C15	4.589135	1.178852	0.453986
F16	5.388238	2.194668	0.117338
F17	4.619138	1.053233	1.805802
F18	5.086671	0.050606	-0.07296
H19	1.529268	3.177682	-0.66697
C20	-5.10584	-1.53368	3.465554
C21	-4.76698	-2.35199	2.385886
C22	-3.64147	-2.06356	1.61552
C23	-2.84433	-0.95513	1.93357
C24	-3.18397	-0.13595	3.02024
C25	-4.31628	-0.42548	3.779593
H26	-5.98558	-1.75893	4.061264
H27	-5.38008	-3.21431	2.141637
H28	-3.37833	-2.69447	0.771312
H29	-2.56556	0.724392	3.259405
H30	-4.58097	0.214091	4.616312
C31	1.426218	-2.04971	5.076097
C32	0.14354	-2.49888	4.740906
C33	-0.48519	-2.05388	3.586618
C34	0.17673	-1.13445	2.735319
C35	1.485491	-0.71225	3.063926
C36	2.093243	-1.16166	4.228558
H37	1.90531	-2.4024	5.984655
H38	-0.36732	-3.20977	5.383592
H39	-1.46566	-2.43186	3.332606
H40	2.011143	-0.05062	2.386144
H41	3.096206	-0.82244	4.468645
C42	-4.63097	0.752053	-2.90714
C43	-4.93331	0.770749	-1.54054
C44	-3.96974	0.445303	-0.59613
C45	-2.66788	0.088873	-1.01972

C46	-2.36247	0.101203	-2.39845
C47	-3.34071	0.422526	-3.32897
H48	-5.39389	1.011719	-3.63512
H49	-5.92693	1.056751	-1.2085
H50	-4.21077	0.499184	0.456446
H51	-1.34922	-0.10977	-2.71195
H52	-3.08571	0.433123	-4.38393
O53	-0.41138	2.285732	0.525564
C54	-0.29673	3.365675	-0.05263
O55	0.71383	3.821778	-0.70717
C56	-1.49719	4.337522	0.006696
F57	-1.30416	5.451619	-0.70301
F58	-2.59632	3.716345	-0.46094
F59	-1.72709	4.681698	1.288758
C60	0.899717	-1.73332	-0.79464
H61	1.704602	-2.04985	-0.12876
H62	0.031987	-2.3923	-0.71279
H63	1.26301	-1.65326	-1.81773

Table S17. $Rh^{II}(NN)(TFA)(TFAH)$

Atom	x	y	z
Rh1	0.145596	0.091317	-0.00793
N2	-0.79722	-0.4243	1.722997
C3	3.049216	0.720028	0.835957
O4	3.656969	-0.11471	0.081803
C5	-1.85142	-0.97127	1.09327
O6	1.85975	1.066268	0.806812
N7	-1.63967	-0.8451	-0.22775
C8	1.646894	-0.19135	-2.58523
O9	0.656864	0.364523	-2.03696
O10	2.663037	-0.7078	-2.06639
C11	1.532797	-0.30725	-4.12585
F12	2.721728	-0.50953	-4.70408
F13	0.738557	-1.36576	-4.42253
F14	0.979118	0.788215	-4.664
C15	3.967861	1.367257	1.896887
F16	4.679432	0.427375	2.5346
F17	4.819859	2.217163	1.298118
F18	3.253318	2.048947	2.801247
H19	3.110144	-0.40942	-0.80988

C20	-5.26262	-2.75076	2.964979
C21	-4.6717	-3.36972	1.861488
C22	-3.56424	-2.79197	1.244769
C23	-3.03192	-1.59147	1.739086
C24	-3.62509	-0.97652	2.852363
C25	-4.73957	-1.55313	3.456971
H26	-6.12944	-3.20078	3.440625
H27	-5.07495	-4.30269	1.478853
H28	-3.10703	-3.26898	0.383536
H29	-3.21379	-0.04774	3.235148
H30	-5.19884	-1.06786	4.313176
C31	0.707046	-1.0833	5.59876
C32	0.004286	-2.10322	4.953528
C33	-0.50936	-1.9109	3.67314
C34	-0.33609	-0.67438	3.025886
C35	0.385683	0.343687	3.671566
C36	0.900685	0.137248	4.94773
H37	1.110125	-1.24289	6.594619
H38	-0.13497	-3.06276	5.443957
H39	-1.03138	-2.71759	3.17055
H40	0.544323	1.283704	3.154698
H41	1.459392	0.932689	5.432435
C42	-4.36449	-0.99347	-3.43245
C43	-4.78455	-0.49836	-2.1961
C44	-3.90216	-0.43972	-1.12012
C45	-2.5808	-0.89602	-1.27114
C46	-2.15595	-1.37366	-2.52122
C47	-3.045	-1.42318	-3.59042
H48	-5.05654	-1.03265	-4.26869
H49	-5.80352	-0.14322	-2.06916
H50	-4.22935	-0.03363	-0.16921
H51	-1.12749	-1.69057	-2.64668
H52	-2.70117	-1.79447	-4.55147

Table S18. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.430631	0.369648	-0.31019
N2	-0.5204	0.162674	1.519811
C3	3.543592	0.765217	-0.13091
O4	3.957031	-0.18943	-0.86788

C5	-1.66523	-0.25133	0.935829
O6	2.400348	1.007437	0.283872
N7	-1.5515	-0.06721	-0.3734
C8	0.729273	1.139095	-3.08609
O9	1.119749	0.213416	-2.33007
O10	0.116498	2.176051	-2.72589
C11	0.991244	0.934739	-4.59309
F12	0.133489	0.004855	-5.06003
F13	0.810375	2.063171	-5.28497
F14	2.241347	0.498645	-4.79924
C15	4.674525	1.736962	0.283493
F16	5.264667	2.239915	-0.81297
F17	4.199337	2.750888	1.014128
F18	5.598993	1.084471	1.005832
H19	0.031492	2.101895	-1.40975
C20	-4.97571	-1.94828	3.041809
C21	-4.60539	-2.46216	1.797272
C22	-3.53694	-1.90457	1.099479
C23	-2.82458	-0.82917	1.651726
C24	-3.19496	-0.32059	2.905548
C25	-4.27063	-0.8769	3.593454
H26	-5.8108	-2.38461	3.582652
H27	-5.14733	-3.30087	1.370338
H28	-3.24274	-2.30772	0.136065
H29	-2.63959	0.507556	3.334242
H30	-4.55608	-0.4765	4.561823
C31	1.330696	-1.3837	4.971925
C32	0.682891	-2.2535	4.092272
C33	0.064121	-1.76582	2.943516
C34	0.072114	-0.38588	2.677432
C35	0.736163	0.483984	3.555409
C36	1.360534	-0.01481	4.695784
H37	1.818121	-1.77163	5.861836
H38	0.671889	-3.32149	4.291804
H39	-0.39688	-2.44582	2.236359
H40	0.752798	1.546191	3.330832
H41	1.870377	0.666578	5.370972
C42	-4.41061	-0.0016	-3.45281
C43	-4.69011	0.616663	-2.23256
C44	-3.75161	0.606178	-1.20335

C45	-2.52506	-0.05304	-1.38464
C46	-2.24116	-0.67053	-2.61194
C47	-3.18178	-0.63829	-3.63871
H48	-5.14168	0.020827	-4.25557
H49	-5.63888	1.124559	-2.08305
H50	-3.95931	1.105265	-0.26225
H51	-1.28742	-1.17047	-2.74518
H52	-2.95106	-1.11416	-4.58735
O60	0.638852	-1.72928	-0.19014
C61	1.513555	-2.47291	-0.71454
O62	2.631532	-2.198	-1.19081
C63	1.070559	-3.95773	-0.77414
F64	2.060169	-4.76773	-1.15852
F65	0.630702	-4.37007	0.43203
F66	0.052502	-4.08512	-1.6503
H67	3.255416	-1.00309	-1.04459
C62	0.003852	2.594989	-0.13695
H62	0.935916	3.162427	-0.12565
H63	-0.80968	3.192584	-0.56896
H64	-0.30682	2.380785	0.883554

Table S19. [Rh^{III}(NN)(TFA^{eq})($TFAH^{ax}$)(CH_3^{ax}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	0.436906	0.40251	-0.30061
N2	-0.52471	0.180177	1.522281
C3	3.481293	0.738529	-0.12671
O4	3.817204	-0.21149	-0.86957
C5	-1.66124	-0.25484	0.93528
O6	2.348268	1.065478	0.311484
N7	-1.54668	-0.08368	-0.37595
C8	0.747958	1.154943	-3.07607
O9	1.124299	0.223966	-2.31712
O10	0.140088	2.194273	-2.72069
C11	1.025896	0.946683	-4.57987
F12	0.19614	-0.00996	-5.04581
F13	0.819453	2.063851	-5.28205
F14	2.288212	0.541913	-4.77482
C15	4.654698	1.650341	0.315675
F16	5.262286	2.16531	-0.76795
F17	4.244301	2.665881	1.087568

F18	5.558859	0.934459	1.006819
H19	0.030114	2.107218	-1.38035
C20	-4.95469	-1.98008	3.044647
C21	-4.58078	-2.49055	1.799859
C22	-3.51789	-1.92319	1.101779
C23	-2.81462	-0.84159	1.653597
C24	-3.18895	-0.33628	2.907513
C25	-4.25917	-0.90231	3.595804
H26	-5.78542	-2.42399	3.585908
H27	-5.11572	-3.33367	1.372839
H28	-3.22146	-2.32271	0.137474
H29	-2.64101	0.497074	3.335681
H30	-4.54786	-0.50449	4.564202
C31	1.366698	-1.31829	4.973914
C32	0.695963	-2.19823	4.122288
C33	0.062871	-1.72614	2.974869
C34	0.078228	-0.35147	2.681931
C35	0.76501	0.52828	3.532264
C36	1.404155	0.044638	4.670817
H37	1.866395	-1.69379	5.862225
H38	0.678192	-3.26206	4.342531
H39	-0.41967	-2.41554	2.291117
H40	0.791628	1.585096	3.285253
H41	1.933104	0.733661	5.323043
C42	-4.40062	0.001238	-3.46128
C43	-4.69352	0.590876	-2.23013
C44	-3.76034	0.571903	-1.19616
C45	-2.52338	-0.06567	-1.38411
C46	-2.22635	-0.65294	-2.62354
C47	-3.16228	-0.61419	-3.65399
H48	-5.12789	0.030503	-4.26713
H49	-5.64924	1.083804	-2.07552
H50	-3.97983	1.05039	-0.24714
H51	-1.2631	-1.13189	-2.76553
H52	-2.91912	-1.06604	-4.61124
O60	0.706177	-1.72324	-0.17172
C61	1.496592	-2.4953	-0.74503
O62	2.615509	-2.25724	-1.29116
C63	1.026344	-3.9674	-0.82073
F64	1.996698	-4.7922	-1.21748

F65	0.58306	-4.37249	0.382515
F66	0.004462	-4.05335	-1.69437
H60	3.049413	-1.24016	-1.12928
C62	-0.03906	2.606887	-0.12702
H62	0.890495	3.175028	-0.08343
H63	-0.84187	3.192556	-0.5935
H64	-0.387	2.384521	0.879131

Table S20. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.231167	0.311195	-0.11153
N2	-0.62129	-0.36889	1.679561
C3	3.300703	1.128958	0.05634
O4	3.837768	0.336748	-0.79375
C5	-1.77912	-0.65106	1.081766
O6	2.157238	1.104992	0.526873
N7	-1.69451	-0.31898	-0.21158
C15	4.264881	2.236438	0.541814
F16	3.609937	3.166404	1.243726
F17	5.213082	1.695291	1.324734
F18	4.858714	2.825846	-0.50548
H19	0.724481	1.897196	-1.54943
C20	-5.24535	-2.29024	2.974791
C21	-4.91657	-2.67686	1.674117
C22	-3.78961	-2.14672	1.050394
C23	-2.97679	-1.22966	1.733129
C24	-3.30685	-0.84892	3.042383
C25	-4.44022	-1.37543	3.656476
H26	-6.12789	-2.70142	3.456817
H27	-5.53867	-3.39211	1.144009
H28	-3.53148	-2.44717	0.040154
H29	-2.67806	-0.1373	3.56768
H30	-4.69538	-1.07111	4.667331
C31	1.20241	-2.1965	4.997604
C32	0.479116	-2.97678	4.093517
C33	-0.13046	-2.39292	2.985052
C34	-0.0399	-1.00476	2.787329
C35	0.703075	-0.22451	3.687687
C36	1.317874	-0.82028	4.785344
H37	1.681845	-2.6588	5.855681

H38	0.400863	-4.05034	4.241887
H39	-0.66118	-3.00332	2.262238
H40	0.782321	0.843784	3.51039
H41	1.887467	-0.20797	5.47893
C42	-4.70419	0.61735	-2.9919
C43	-4.73142	1.198264	-1.72238
C44	-3.73891	0.903302	-0.78974
C45	-2.71658	-0.00012	-1.1201
C46	-2.6882	-0.5803	-2.39833
C47	-3.67803	-0.26938	-3.32719
H48	-5.47626	0.856753	-3.71738
H49	-5.52336	1.893742	-1.45903
H50	-3.74379	1.366271	0.191972
H51	-1.89201	-1.27792	-2.63879
H52	-3.65178	-0.72547	-4.31285
O53	-0.44854	2.204827	0.450426
C54	0.010007	3.168889	-0.20769
O55	0.714466	3.085666	-1.25325
C56	-0.33371	4.577662	0.317912
F57	-1.66709	4.742906	0.316514
F58	0.112025	4.711708	1.576179
F59	0.216701	5.531139	-0.43726
O60	0.646449	-1.69952	-0.41542
C61	1.682577	-2.28601	-0.83883
O62	2.780729	-1.82797	-1.20518
C63	1.486913	-3.82313	-0.92827
F64	2.615021	-4.45177	-1.26946
F65	1.068388	-4.31335	0.253584
F66	0.547158	-4.10589	-1.85299
H67	3.268348	-0.54663	-0.99504
C62	0.650203	0.719348	-2.34986
H62	0.806334	-0.35353	-2.44376
H63	-0.2511	0.982172	-2.91014
H64	1.525828	1.170413	-2.83782

Table S21. [Rh^{III}(NN)(TFA^{ax})($TFAH^{ax}$)(CH_3^{eq}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	0.238667	0.516753	-0.14525
N2	-0.60226	-0.18617	1.652851
C3	3.12489	0.943379	-0.22815

O4	2.982373	0.777591	-1.46456
C5	-1.7527	-0.52032	1.044495
O6	2.171484	1.127141	0.584912
N7	-1.71188	-0.13113	-0.2272
C15	4.553997	1.045765	0.337083
F16	4.836442	2.36122	0.490774
F17	4.640322	0.457087	1.529789
F18	5.450065	0.511919	-0.48947
H19	1.631459	2.365175	1.467836
C20	-5.01335	-2.51638	2.967337
C21	-4.69691	-2.82143	1.642155
C22	-3.64312	-2.16956	1.005645
C23	-2.89011	-1.21057	1.69922
C24	-3.20869	-0.91146	3.032506
C25	-4.26918	-1.55955	3.660221
H26	-5.83689	-3.02538	3.46036
H27	-5.27013	-3.57026	1.103411
H28	-3.39315	-2.41057	-0.02226
H29	-2.62337	-0.17268	3.570347
H30	-4.51255	-1.32039	4.691381
C31	1.332738	-2.22446	4.790582
C32	0.676257	-2.95231	3.796618
C33	0.027957	-2.29751	2.751977
C34	0.015036	-0.89313	2.703683
C35	0.686805	-0.16582	3.698183
C36	1.339838	-0.82908	4.733535
H37	1.845939	-2.74095	5.596549
H38	0.683313	-4.0385	3.822299
H39	-0.44392	-2.86532	1.957555
H40	0.685747	0.919304	3.649109
H41	1.856575	-0.25506	5.497633
C42	-4.85689	0.516417	-2.93999
C43	-4.92487	1.061688	-1.65618
C44	-3.88639	0.862456	-0.74958
C45	-2.7747	0.08831	-1.11799
C46	-2.70375	-0.4546	-2.41053
C47	-3.74186	-0.2369	-3.31412
H48	-5.66628	0.680678	-3.64538
H49	-5.78622	1.654417	-1.36093
H50	-3.92663	1.29873	0.243481

H51	-1.84007	-1.05533	-2.67922
H52	-3.6827	-0.66445	-4.31105
O53	-0.51001	2.470016	0.346018
C54	-0.04195	3.236943	1.184033
O55	1.096269	3.144055	1.808282
C56	-0.83606	4.496974	1.591797
F57	-0.18115	5.591698	1.176721
F58	-2.05115	4.482926	1.045291
F59	-0.95666	4.545099	2.926004
O60	0.662929	-1.39823	-0.65057
C61	1.757944	-2.02409	-0.3523
O62	2.796813	-1.62223	0.145711
C63	1.619816	-3.52247	-0.74623
F64	2.714061	-4.21725	-0.4194
F65	0.563995	-4.0902	-0.11781
F66	1.420327	-3.65179	-2.07371
H67	1.778353	0.851381	-1.68725
C62	0.543807	1.251387	-2.29652
H62	-0.52622	1.094487	-2.42601
H63	0.745293	2.323865	-2.38344
H64	1.002497	0.722378	-3.14356

Table S22. [$Rh^{III\text{-}I}$(NN)(TFA^{eq})($TFAH^{ax}$)($TFAH^{eq}$)(CH_3^{ax}-TFA)]$^{-‡}$

Atom	x	y	z
Rh1	-0.59529	1.16605	-3.0324
N2	-1.55619	-0.32208	-1.95801
C3	2.223921	0.873858	-1.92683
O4	1.953376	1.24759	-0.75902
C5	-2.78061	0.183317	-2.17942
O6	1.490187	0.741503	-2.93485
N7	-2.6662	1.265401	-2.94858
C8	0.690853	3.833912	-3.87951
O9	0.052305	2.85232	-4.23378
O10	0.918243	4.278022	-2.67599
C11	1.353524	4.735775	-4.94111
F12	0.824759	5.973778	-4.89391
F13	2.674332	4.837454	-4.70464
F14	1.176454	4.246174	-6.16863
C15	3.707646	0.506644	-2.19248
F16	3.819676	-0.79279	-2.53556

F17	4.204258	1.24381	-3.20814
F18	4.48956	0.713988	-1.11986
H19	0.715729	1.5729	-0.16315
C20	-6.4532	-1.38537	-0.61519
C21	-6.37724	-0.98171	-1.94948
C22	-5.18702	-0.4659	-2.45897
C23	-4.0556	-0.35764	-1.63701
C24	-4.1384	-0.76255	-0.29654
C25	-5.33238	-1.27124	0.209811
H26	-7.38284	-1.78653	-0.21929
H27	-7.24608	-1.06823	-2.59653
H28	-5.12597	-0.1499	-3.4957
H29	-3.26637	-0.66704	0.34198
H30	-5.38775	-1.57877	1.250789
C31	-0.44885	-4.19277	-0.70005
C32	-1.5799	-4.02202	-1.50004
C33	-1.96437	-2.75284	-1.92702
C34	-1.22772	-1.61513	-1.54206
C35	-0.081	-1.7979	-0.74709
C36	0.299024	-3.07111	-0.33312
H37	-0.14748	-5.18582	-0.37708
H38	-2.16248	-4.88613	-1.81113
H39	-2.82998	-2.63656	-2.57067
H40	0.496889	-0.92726	-0.45742
H41	1.187628	-3.1867	0.282928
C42	-5.46412	4.318341	-3.71225
C43	-5.24894	3.890516	-2.40116
C44	-4.33195	2.876658	-2.12993
C45	-3.62378	2.264975	-3.179
C46	-3.83798	2.700161	-4.499
C47	-4.75336	3.71858	-4.75546
H48	-6.1751	5.114313	-3.91906
H49	-5.78709	4.356374	-1.57891
H50	-4.14752	2.562032	-1.10833
H51	-3.30501	2.213817	-5.31234
H52	-4.91526	4.039762	-5.78132
O53	-0.56674	3.684566	-0.64054
C54	-0.77181	2.832626	0.21771
O55	-0.11316	1.757094	0.480758
C56	-0.76407	0.050687	-5.18584

H57	-1.50397	-0.62938	-4.79734
H58	-1.07148	1.012272	-5.55954
H59	0.280642	-0.21513	-5.12534
H60	0.388153	3.820659	-1.94904
O61	-0.89133	-0.7371	-6.95026
C62	-1.79023	-0.17014	-7.66119
O63	-2.56757	0.746242	-7.39451
C64	-1.87984	-0.74171	-9.10822
F65	-1.10842	-1.82616	-9.31796
F66	-3.15174	-1.09203	-9.40679
F67	-1.50323	0.197449	-10.0081
C68	-1.97906	3.000634	1.171078
F69	-1.56984	3.057724	2.453728
F70	-2.66743	4.114439	0.901318
F71	-2.82013	1.950363	1.05212

Table S23. [$Rh^{III\text{-}I}$(NN)(TFA^{eq})($TFAH^{ax}$)($TFAH^{eq}$)(CH_3^{ax}-TFAH)]‡

Atom	x	y	z
Rh1	0.258603	0.059931	-0.17903
N2	-0.60126	-0.19115	1.673844
C3	3.515956	0.149569	0.442979
O4	4.008259	-1.02667	0.33445
C5	-1.84425	-0.2938	1.182344
O6	2.362608	0.563957	0.265544
N7	-1.77506	-0.15679	-0.14913
C8	0.663846	1.042064	-3.09691
O9	0.744998	0.124167	-2.28588
O10	0.402138	2.295206	-2.87484
C11	0.881001	0.705131	-4.58722
F12	0.933112	1.797074	-5.35226
F13	2.027671	0.023166	-4.72443
F14	-0.13113	-0.07214	-5.00775
C15	4.597055	1.165039	0.891907
F16	4.15408	2.422903	0.733334
F17	4.879849	0.974957	2.189573
F18	5.716576	1.016101	0.177027
H19	1.729232	2.229522	0.765936
C20	-5.37627	-0.99263	3.499839
C21	-5.21949	-1.61669	2.260464
C22	-4.07609	-1.38472	1.499958

C23	-3.0714	-0.53016	1.979546
C24	-3.23302	0.091555	3.227392
C25	-4.38298	-0.1368	3.979608
H26	-6.27016	-1.17318	4.090359
H27	-5.98897	-2.28544	1.88567
H28	-3.95378	-1.86742	0.535481
H29	-2.45842	0.754415	3.599895
H30	-4.50285	0.352868	4.941789
C31	1.025677	-1.72817	5.249923
C32	0.052731	-2.4574	4.563793
C33	-0.5047	-1.96624	3.384029
C34	-0.10408	-0.71619	2.877922
C35	0.881798	0.010127	3.56911
C36	1.437826	-0.49306	4.742846
H37	1.462143	-2.11977	6.163836
H38	-0.26847	-3.42483	4.940366
H39	-1.24776	-2.54824	2.848221
H40	1.186305	0.977003	3.17967
H41	2.194292	0.085439	5.266297
C42	-4.68775	1.075402	-2.93414
C43	-4.74659	1.544547	-1.62048
C44	-3.79562	1.152226	-0.68143
C45	-2.77245	0.256835	-1.04298
C46	-2.70938	-0.20118	-2.37088
C47	-3.65947	0.205991	-3.3041
H48	-5.4282	1.39194	-3.66289
H49	-5.53179	2.235201	-1.32434
H50	-3.83605	1.542868	0.329707
H51	-1.90914	-0.87781	-2.65508
H52	-3.59554	-0.15971	-4.32542
O53	0.101876	3.497837	-0.53541
C54	0.504421	3.699059	0.593994
O55	1.403684	3.017668	1.265945
C56	-0.0398	4.872522	1.441466
F57	0.969101	5.663798	1.838578
F58	-0.9056	5.597249	0.733831
F59	-0.6619	4.39238	2.53127
C60	0.69124	-2.36754	-0.35169
H61	1.242026	-2.0271	-1.21356
H62	1.079115	-2.24305	0.646744

H63	-0.35185	-2.61824	-0.47051
H64	0.277936	2.519133	-1.90968
O65	1.267549	-4.10923	-0.51654
C66	2.532756	-4.19177	-0.47975
O67	3.378648	-3.29613	-0.30125
C68	3.055425	-5.63463	-0.71232
F69	2.532613	-6.47081	0.202315
F70	2.685598	-6.06272	-1.93368
F71	4.388619	-5.69859	-0.62906
H72	3.486198	-1.89204	0.044793

Table S24. $[Rh^{III\text{-}II}(NN)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{\ddagger}$

Atom	x	y	z
Rh1	-0.66913	-2.16534	-2.78933
N2	-1.29833	-4.02651	-2.3283
C3	-1.73276	-1.88826	-5.63769
O4	-0.99468	-2.74	-6.17249
C5	-0.44736	-4.17597	-1.29302
O6	-1.81092	-1.53082	-4.42694
N7	0.265036	-3.03295	-1.23233
C8	0.826549	0.333667	-3.76411
O9	0.160925	-0.19362	-2.87324
O10	1.456166	-0.24627	-4.73838
C11	0.978557	1.871835	-3.79287
F12	0.450868	2.344828	-4.93037
F13	0.362121	2.424078	-2.75472
F14	2.282155	2.191552	-3.75433
C15	-2.70891	-1.11188	-6.55985
F16	-2.69314	-1.58474	-7.81041
F17	-3.96411	-1.19989	-6.08831
F18	-2.3573	0.186916	-6.59121
H19	0.004672	-3.61245	-5.64392
C20	-0.17532	-7.54605	1.310016
C21	-0.16908	-6.25402	1.840135
C22	-0.24496	-5.15118	0.993412
C23	-0.3399	-5.34189	-0.39458
C24	-0.34863	-6.64147	-0.9245
C25	-0.26148	-7.73775	-0.07073
H26	-0.11291	-8.40382	1.973397
H27	-0.10637	-6.10393	2.913656

H28	-0.24358	-4.14636	1.404493
H29	-0.40904	-6.78616	-1.99818
H30	-0.26059	-8.74212	-0.4833
C31	-4.90188	-6.00061	-3.18042
C32	-4.54155	-5.77305	-1.84956
C33	-3.33772	-5.14737	-1.54286
C34	-2.48259	-4.73669	-2.58322
C35	-2.85246	-4.953	-3.92138
C36	-4.05361	-5.59084	-4.21232
H37	-5.84559	-6.48519	-3.4119
H38	-5.2081	-6.06988	-1.04547
H39	-3.0705	-4.9506	-0.51045
H40	-2.18852	-4.62676	-4.71433
H41	-4.33175	-5.762	-5.24774
C42	3.804912	-2.12419	0.819638
C43	3.648182	-3.39305	0.253032
C44	2.476937	-3.7259	-0.41801
C45	1.448275	-2.77133	-0.52782
C46	1.612179	-1.48755	0.023866
C47	2.784881	-1.17595	0.703708
H48	4.722891	-1.87385	1.343153
H49	4.448641	-4.12349	0.323684
H50	2.365618	-4.69733	-0.88472
H51	0.811456	-0.75949	-0.06317
H52	2.900576	-0.19051	1.144318
O53	1.993783	-2.77846	-4.39875
C54	1.693219	-3.93577	-4.68033
O55	0.677341	-4.36787	-5.34805
C56	2.563429	-5.09715	-4.14553
F57	3.708116	-4.64999	-3.62978
F58	1.874882	-5.72932	-3.15884
F59	2.832981	-5.99078	-5.10231
C60	-2.49641	-1.28559	-1.56624
H61	-2.53886	-0.44406	-2.24308
H62	-3.14406	-2.13194	-1.73619
H63	-1.86088	-1.24806	-0.69334
H64	1.493733	-1.2487	-4.6569
O65	-3.93237	-0.4886	-0.43452
V66	-3.64989	0.953846	0.290711
Cl67	-5.17375	1.752283	1.656019

Cl68	-1.68933	0.662407	1.346498
Cl69	-3.13293	2.387867	-1.32688

Table S25. [Rh^{IV-II}(NN)(TFA^{eq})($TFAH^{ax}$)($TFAH^{eq}$)(CH_3^{ax}-TFA)]‡

Atom	x	y	z
Rh1	0.371839	0.020798	-0.16217
N2	-0.42484	-0.42264	1.659944
C3	3.470555	0.523284	0.051731
O4	3.806563	-0.22727	-0.86964
C5	-1.65082	-0.65962	1.164934
O6	2.288398	0.878189	0.390705
N7	-1.56825	-0.5928	-0.16973
C8	1.35217	-0.10704	-3.175
O9	0.607423	0.351815	-2.30296
O10	2.555034	-0.55498	-3.0517
C11	0.860243	-0.08859	-4.64041
F12	1.42952	-1.05047	-5.36534
F13	-0.46691	-0.22104	-4.69376
F14	1.19171	1.106145	-5.17536
C15	4.57253	1.112087	0.968233
F16	5.794545	0.899787	0.484131
F17	4.389426	2.442958	1.107649
F18	4.487259	0.553183	2.191225
H19	1.853571	2.332854	0.953212
C20	-5.22265	-1.35656	3.406135
C21	-5.01171	-2.0322	2.202507
C22	-3.84886	-1.80911	1.469481
C23	-2.88099	-0.91148	1.946128
C24	-3.09381	-0.23962	3.159979
C25	-4.26388	-0.45956	3.881881
H26	-6.13368	-1.52806	3.972434
H27	-5.7548	-2.73222	1.832389
H28	-3.68536	-2.33013	0.531694
H29	-2.34745	0.457377	3.527457
H30	-4.42787	0.070123	4.815665
C31	1.32867	-1.70735	5.262436
C32	0.326122	-2.47706	4.669089
C33	-0.26323	-2.07236	3.474393
C34	0.135212	-0.86704	2.867697
C35	1.154229	-0.10249	3.459836

C36	1.74381	-0.52374	4.647746
H37	1.789725	-2.03265	6.190266
H38	0.008641	-3.40785	5.1306
H39	-1.02779	-2.68512	3.008884
H40	1.476224	0.814042	2.979117
H41	2.531371	0.076016	5.094521
C42	-4.50869	0.383769	-3.00514
C43	-4.48086	1.060775	-1.78332
C44	-3.51521	0.750164	-0.83042
C45	-2.57753	-0.26212	-1.09436
C46	-2.5919	-0.93041	-2.32813
C47	-3.56	-0.60546	-3.27463
H48	-5.25964	0.635359	-3.74861
H49	-5.20464	1.84418	-1.57677
H50	-3.46841	1.295056	0.106535
H51	-1.84319	-1.68928	-2.53451
H52	-3.56812	-1.12397	-4.22878
O53	-0.4371	2.237054	0.246655
C54	0.131768	3.140103	0.841746
O55	1.378308	3.175559	1.232728
C56	-0.62538	4.432192	1.224841
F57	-0.1025	5.481455	0.572704
F58	-1.91853	4.327575	0.910366
F59	-0.51906	4.650695	2.5456
C60	1.070498	-2.05769	-0.30516
H61	2.145238	-1.96837	-0.22661
H62	0.570956	-2.5986	0.486509
H63	0.585117	-1.9956	-1.28498
H64	2.954447	-0.45731	-2.1119
O65	1.426987	-3.94811	-1.27042
C66	0.960126	-3.87134	-2.45343
O67	0.376865	-2.94071	-3.01874
C68	1.199263	-5.19679	-3.24924
F69	0.638077	-6.23749	-2.60526
F70	0.670204	-5.13217	-4.4765
F71	2.516887	-5.43851	-3.36998

Table S26. [$Rh^{IV\text{-}II}(NN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-\ddagger}$

Atom	x	y	z
Rh1	0.578732	0.469639	-0.13349

N2	-0.15296	-0.64484	1.429033
C3	3.43889	1.379847	0.469969
O4	3.242884	2.600966	0.576582
C5	-1.40566	-0.69566	0.939966
O6	2.63936	0.424105	0.255431
N7	-1.44786	0.005545	-0.18893
C8	0.501543	2.513769	-2.36388
O9	1.114714	1.494019	-1.88849
O10	-0.45654	3.148321	-1.9284
C11	1.143976	2.967893	-3.70537
F12	0.499868	4.019989	-4.23985
F13	2.434212	3.328519	-3.52917
F14	1.121927	1.973231	-4.62028
C15	4.905049	0.890411	0.6122
F16	5.71764	1.847836	1.085653
F17	4.984036	-0.16498	1.451833
F18	5.38465	0.495585	-0.58526
H19	1.98443	3.388402	0.464775
C20	-4.68183	-2.86424	2.638754
C21	-3.48929	-3.52304	2.332825
C22	-2.41944	-2.82092	1.780509
C23	-2.54619	-1.44758	1.528416
C24	-3.74905	-0.79035	1.81897
C25	-4.81143	-1.49861	2.378637
H26	-5.51249	-3.41624	3.071536
H27	-3.39238	-4.58973	2.515667
H28	-1.50434	-3.33355	1.5017
H29	-3.84378	0.270693	1.60728
H30	-5.74116	-0.98466	2.607671
C31	1.351616	-1.45828	5.276061
C32	0.00928	-1.10629	5.124336
C33	-0.51518	-0.82538	3.865394
C34	0.30277	-0.91449	2.722211
C35	1.661194	-1.24768	2.882861
C36	2.173466	-1.51691	4.14783
H37	1.7554	-1.67085	6.262422
H38	-0.63703	-1.03473	5.995866
H39	-1.552	-0.52694	3.765885
H40	2.302732	-1.26822	2.008841
H41	3.225029	-1.77188	4.250536

C42	-4.40125	-0.14755	-3.17515
C43	-3.90793	1.078874	-2.72223
C44	-2.92718	1.125865	-1.73471
C45	-2.43959	-0.06905	-1.18434
C46	-2.91216	-1.30637	-1.65675
C47	-3.89533	-1.33574	-2.64387
H48	-5.16504	-0.17738	-3.94828
H49	-4.28468	2.007386	-3.14328
H50	-2.51626	2.067311	-1.38802
H51	-2.4858	-2.22764	-1.2711
H52	-4.2556	-2.29447	-3.00822
O53	-0.19229	2.411435	1.000448
C54	0.065598	3.569312	0.689677
O55	1.221247	4.088311	0.420652
C56	-1.0674	4.617937	0.719892
F57	-0.86222	5.631919	-0.12612
F58	-2.25197	4.05702	0.441538
F59	-1.14447	5.13369	1.973311
C60	0.817457	-1.29843	-1.52623
H61	1.889381	-1.20777	-1.64004
H62	0.390101	-1.91325	-0.74381
H63	0.194951	-0.98861	-2.35214
O64	0.962481	-3.22884	-2.43286
C65	0.201356	-4.03134	-1.80961
O66	-0.52544	-3.8599	-0.82248
C67	0.257092	-5.48268	-2.38573
F68	1.247053	-6.18028	-1.77921
F69	-0.89445	-6.1475	-2.16697
F70	0.494655	-5.51485	-3.71095

Table S27. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_2TFA^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.595531	0.511725	-0.56179
N2	-0.42966	0.528211	1.237461
C3	3.754184	0.715012	-0.34299
O4	4.119267	-0.31953	-0.99544
C5	-1.57659	0.126204	0.642202
O6	2.619585	1.053303	0.023351
N7	-1.39792	0.1789	-0.66789
C8	0.866345	1.090773	-3.36747

O9	1.312925	0.227728	-2.56804
O10	0.229196	2.129392	-3.05023
C11	1.078138	0.817694	-4.87265
F12	0.061189	0.058781	-5.32322
F13	1.102394	1.957403	-5.57292
F14	2.225429	0.161099	-5.08428
C15	4.938047	1.643031	0.0218
F16	5.579626	2.017253	-1.09658
F17	4.512943	2.739007	0.657402
F18	5.802023	0.993122	0.815699
H19	0.261201	2.183939	-1.71489
C20	-5.08403	-1.11649	2.743537
C21	-4.74137	-1.7337	1.539274
C22	-3.60822	-1.32522	0.840678
C23	-2.80252	-0.2961	1.352863
C24	-3.14845	0.318954	2.566401
C25	-4.28798	-0.08959	3.253778
H26	-5.96991	-1.43662	3.284739
H27	-5.35557	-2.53711	1.143615
H28	-3.33861	-1.81162	-0.09037
H29	-2.53173	1.118496	2.960707
H30	-4.55356	0.394149	4.189028
C31	1.200854	-0.85831	4.862541
C32	0.587015	-1.76521	3.995685
C33	0.037406	-1.32959	2.792364
C34	0.085787	0.034348	2.457031
C35	0.710543	0.943647	3.324385
C36	1.263179	0.494596	4.521449
H37	1.633779	-1.20566	5.796332
H38	0.546431	-2.82052	4.250887
H39	-0.40221	-2.03798	2.099102
H40	0.737964	1.994624	3.053799
H41	1.74051	1.204426	5.191027
C42	-4.07595	-0.08773	-3.88915
C43	-4.22867	0.925719	-2.94088
C44	-3.34415	1.028134	-1.86891
C45	-2.31234	0.088156	-1.73509
C46	-2.1533	-0.93042	-2.68565
C47	-3.0355	-1.01076	-3.76076
H48	-4.7624	-0.15473	-4.72815

H49	-5.03187	1.650254	-3.0415
H50	-3.43455	1.8299	-1.14468
H51	-1.35501	-1.65434	-2.55726
H52	-2.91286	-1.80019	-4.49639
O60	0.641733	-1.56067	-0.31954
C61	1.473248	-2.3926	-0.78759
O62	2.61587	-2.22637	-1.24598
C63	0.908344	-3.83696	-0.79106
F64	1.838592	-4.7433	-1.09571
F65	0.386022	-4.14969	0.410474
F66	-0.08237	-3.92177	-1.70703
H67	3.36264	-1.06849	-1.1439
C62	0.38571	2.797429	-0.49647
H62	0.864618	3.582306	-1.09771
H64	0.96913	2.728618	0.418295
O64	-0.9561	3.241948	-0.19949
C65	-1.1553	3.778531	1.003258
O66	-0.3425	3.960774	1.875949
C67	-2.6317	4.192708	1.201976
F68	-3.4087	3.925407	0.139591
F69	-3.13509	3.53927	2.264781
F70	-2.69424	5.508314	1.448534

Table S28. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{ax})]^{\ddagger}$

Atom	x	y	z
Rh1	0.125954	0.748994	-0.4426
N2	-0.41794	-0.30109	1.266443
C3	3.235526	1.316687	-0.02647
O4	3.730827	0.135122	-0.0233
C5	-1.61962	-0.61086	0.777254
O6	2.052898	1.672482	-0.04743
N7	-1.72731	-0.07194	-0.43774
C15	4.321383	2.4171	0.048225
F16	3.812446	3.61088	-0.26742
F17	4.804076	2.475667	1.303266
F18	5.330315	2.142106	-0.78587
H19	0.220406	2.590098	-1.64244
C20	-4.69267	-2.74959	2.843679
C21	-4.40482	-3.06613	1.514908
C22	-3.40421	-2.37821	0.830785

C23	-2.67986	-1.37046	1.482993
C24	-2.96655	-1.05973	2.821082
C25	-3.97328	-1.7458	3.495098
H26	-5.47621	-3.28536	3.372196
H27	-4.96029	-3.85057	1.009436
H28	-3.17577	-2.62865	-0.2
H29	-2.40279	-0.28059	3.324262
H30	-4.19509	-1.49754	4.528933
C31	1.728317	-1.81834	4.545562
C32	1.029109	-2.69602	3.714791
C33	0.316903	-2.21607	2.618324
C34	0.277539	-0.83528	2.361848
C35	0.989336	0.045094	3.192054
C36	1.711499	-0.44808	4.275301
H37	2.291949	-2.20079	5.391527
H38	1.053378	-3.76463	3.909143
H39	-0.19248	-2.90107	1.948543
H40	0.956677	1.10869	2.975558
H41	2.259336	0.24001	4.912963
C42	-4.80529	-0.01082	-3.29604
C43	-5.00037	0.60324	-2.05704
C44	-3.98979	0.59102	-1.09675
C45	-2.77996	-0.0642	-1.37006
C46	-2.5861	-0.68986	-2.61245
C47	-3.59649	-0.65441	-3.57077
H48	-5.59129	0.013686	-4.04525
H49	-5.93949	1.104597	-1.84038
H50	-4.12625	1.07955	-0.13681
H51	-1.64957	-1.20557	-2.80116
H52	-3.43965	-1.13636	-4.5315
O53	-0.58967	2.407749	0.596721
C54	-0.43352	3.514637	0.025302
O55	0.027259	3.697005	-1.13494
C56	-0.86485	4.783669	0.789002
F57	-1.24236	4.499733	2.038948
F58	0.150002	5.657426	0.832228
F59	-1.89801	5.355411	0.147952
O60	0.607515	-1.01185	-1.42937
C61	1.339724	-1.94335	-0.96853
O62	2.298786	-1.87925	-0.18528

C63	0.873521	-3.34581	-1.43311
F64	1.824914	-4.26979	-1.29129
F65	-0.18803	-3.71015	-0.66875
F66	0.470022	-3.33331	-2.71254
H67	3.038157	-0.65858	-0.05826
C62	0.374314	1.555534	-2.61774
H63	0.08631	2.405551	-3.25431
H64	-0.22962	0.723619	-2.97553
O64	1.777946	1.289073	-2.85725
C65	2.074333	0.43672	-3.83983
O66	1.326811	-0.03039	-4.66068
C67	3.562617	0.034522	-3.74707
F68	4.327468	1.014001	-3.23876
F69	3.667424	-1.04028	-2.93308
F70	4.033887	-0.30043	-4.94969

Table S29. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{ax})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.349576	0.525942	0.006097
N2	-0.65412	-0.16094	1.693441
C3	3.20039	0.933674	0.106786
O4	3.07044	1.436659	-1.03507
C5	-1.80679	-0.34119	1.090435
O6	2.279968	0.431126	0.8052
N7	-1.8085	0.386265	-0.0866
C15	4.59851	0.956156	0.759931
F16	4.896249	-0.24653	1.270201
F17	5.544465	1.29731	-0.118
F18	4.599722	1.855539	1.762179
H19	-1.91391	1.807552	0.377493
C20	-5.10314	-2.42235	2.863195
C21	-4.66566	-2.79796	1.592877
C22	-3.60166	-2.13147	0.987319
C23	-2.95793	-1.08463	1.663096
C24	-3.39607	-0.71682	2.94656
C25	-4.46826	-1.37833	3.538086
H26	-5.93526	-2.94352	3.327944
H27	-5.15158	-3.61525	1.068213
H28	-3.26537	-2.43511	0.00401
H29	-2.89701	0.089433	3.474756

H30	-4.80445	-1.08091	4.526893
C31	0.967521	-2.12836	5.031649
C32	0.519741	-2.87541	3.940081
C33	-0.03265	-2.24121	2.829462
C34	-0.14597	-0.84405	2.821753
C35	0.3253	-0.09014	3.903326
C36	0.872513	-0.73519	5.009377
H37	1.402683	-2.62949	5.891475
H38	0.612793	-3.95754	3.945651
H39	-0.34167	-2.80912	1.95936
H40	0.260688	0.992968	3.86274
H41	1.233453	-0.14936	5.849644
C42	-4.34049	-0.44813	-3.37305
C43	-4.55152	0.683767	-2.58505
C44	-3.71527	0.953825	-1.50285
C45	-2.66945	0.077347	-1.19084
C46	-2.44715	-1.05428	-1.98951
C47	-3.28446	-1.31121	-3.07493
H48	-4.99082	-0.65309	-4.2186
H49	-5.36522	1.365421	-2.81499
H50	-3.8718	1.844092	-0.9022
H51	-1.62192	-1.7182	-1.75724
H52	-3.10741	-2.19018	-3.68846
O53	0.362209	2.559095	0.572246
C54	-0.6652	3.219653	0.797083
O55	-1.8781	2.81184	0.759485
C56	-0.46421	4.711081	1.143943
F57	-1.61415	5.299568	1.476938
F58	0.394022	4.824106	2.167029
F59	0.053903	5.336682	0.075657
O60	0.340165	-1.45095	-0.4615
C61	1.32722	-2.0077	-1.09708
O62	2.321889	-1.50404	-1.58444
C63	1.076753	-3.53682	-1.21117
F64	2.068979	-4.15356	-1.85453
F65	0.949915	-4.10065	0.009687
F66	-0.0735	-3.77483	-1.88836
H67	1.861294	1.181339	-1.38294
C62	0.798475	1.120979	-2.26265
H62	-0.22974	0.785054	-2.38889

H64	1.436494	0.537549	-2.92973
O64	0.912931	2.492703	-2.73026
C65	-0.12013	3.301859	-2.56935
O66	-1.19136	3.03781	-2.07087
C67	0.21847	4.703305	-3.12825
F68	1.28172	5.221996	-2.49226
F69	0.503151	4.630053	-4.44
F70	-0.82148	5.526038	-2.96385

Table S30. $[Rh^{III}(NN)(TFA^{eq})(TFAH^{ax})(CH_2OH^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.621845	0.577211	-0.57496
N2	-0.44083	0.612785	1.237506
C3	3.684476	0.680225	-0.34876
O4	3.952158	-0.36152	-0.98165
C5	-1.56201	0.121295	0.628636
O6	2.571776	1.157033	0.006138
N7	-1.37037	0.142138	-0.67479
C8	0.876275	1.072115	-3.36592
O9	1.324059	0.214198	-2.55829
O10	0.218354	2.094972	-3.05129
C11	1.115511	0.805387	-4.86656
F12	0.11244	0.037779	-5.33599
F13	1.137697	1.947747	-5.5627
F14	2.271361	0.160455	-5.0657
C15	4.919645	1.521169	0.069252
F16	5.624856	1.868949	-1.02146
F17	4.57502	2.642772	0.718734
F18	5.717102	0.798123	0.874936
H19	0.235692	2.08059	-1.66227
C20	-5.06004	-1.20693	2.70089
C21	-4.68262	-1.8222	1.506154
C22	-3.55141	-1.38655	0.821256
C23	-2.78097	-0.3312	1.334827
C24	-3.16146	0.27888	2.540547
C25	-4.29907	-0.1554	3.215309
H26	-5.94393	-1.54847	3.231995
H27	-5.26787	-2.64538	1.107293
H28	-3.2559	-1.87085	-0.10282
H29	-2.56544	1.089954	2.946455

H30	-4.58972	0.324577	4.145008
C31	1.209807	-0.71087	4.884279
C32	0.569723	-1.62847	4.049066
C33	0.015858	-1.21722	2.838782
C34	0.082796	0.134762	2.461824
C35	0.738024	1.05136	3.298079
C36	1.297083	0.629141	4.501096
H37	1.645916	-1.03949	5.823062
H38	0.511994	-2.67532	4.333956
H39	-0.44406	-1.93881	2.172575
H40	0.801247	2.091857	2.992264
H41	1.8007	1.348147	5.140742
C42	-4.09581	-0.04663	-3.86372
C43	-4.22502	0.951308	-2.89581
C44	-3.32855	1.021308	-1.83158
C45	-2.306	0.068723	-1.72653
C46	-2.16624	-0.92913	-2.70034
C47	-3.06336	-0.98175	-3.76519
H48	-4.79217	-0.09053	-4.69598
H49	-5.01887	1.688451	-2.97565
H50	-3.39399	1.814196	-1.09345
H51	-1.36932	-1.65927	-2.60241
H52	-2.95549	-1.75666	-4.51843
O53	0.7805	-1.58595	-0.23899
C54	1.465905	-2.44939	-0.8075
O55	2.602134	-2.3417	-1.3716
C56	0.840784	-3.8615	-0.88744
F57	1.748372	-4.81119	-1.11814
F58	0.191622	-4.15229	0.251024
F59	-0.05841	-3.87561	-1.89667
H60	3.100254	-1.37898	-1.2357
C61	0.315157	2.855927	-0.43931
H62	0.51135	3.590424	-1.22845
H63	1.157378	2.871971	0.253123
O64	-0.91728	3.14549	0.117947
H65	-0.99404	2.555673	0.887802

Table S31. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_2OH^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.609309	0.552075	-0.56336

N2	-0.44381	0.593545	1.252322
C3	3.746781	0.698782	-0.3782
O4	4.075871	-0.35904	-1.00011
C5	-1.57321	0.129617	0.637617
O6	2.626424	1.088448	-0.00564
N7	-1.3775	0.170092	-0.66375
C8	0.821395	1.072611	-3.35813
O9	1.307978	0.22799	-2.56042
O10	0.150174	2.083834	-3.029
C11	1.07721	0.815397	-4.85783
F12	0.553011	-0.37202	-5.20559
F13	0.528642	1.76299	-5.62337
F14	2.398988	0.784812	-5.09494
C15	4.934918	1.648842	-0.09082
F16	5.137057	2.425987	-1.17277
F17	4.671221	2.44269	0.954797
F18	6.058089	0.968461	0.160716
H19	0.210729	2.095364	-1.67766
C20	-5.10883	-1.12982	2.686914
C21	-4.74245	-1.74787	1.490138
C22	-3.59735	-1.33801	0.811859
C23	-2.80264	-0.30586	1.334982
C24	-3.17177	0.306594	2.543051
C25	-4.32274	-0.10169	3.210953
H26	-6.00393	-1.45084	3.212196
H27	-5.34738	-2.5533	1.084339
H28	-3.31067	-1.82576	-0.11302
H29	-2.55683	1.099997	2.955244
H30	-4.60467	0.380471	4.142237
C31	1.171656	-0.82578	4.879096
C32	0.537308	-1.72057	4.014967
C33	-0.00494	-1.27798	2.810512
C34	0.068438	0.083028	2.468927
C35	0.718175	0.976846	3.333459
C36	1.265355	0.523477	4.53092
H37	1.598371	-1.17924	5.813342
H38	0.475993	-2.77448	4.271944
H39	-0.45366	-1.98237	2.119442
H40	0.784647	2.024776	3.054491
H41	1.763975	1.224974	5.193693

C42	-4.05091	-0.09354	-3.88807
C43	-4.16282	0.956699	-2.97468
C44	-3.28027	1.052866	-1.90066
C45	-2.29299	0.073494	-1.73149
C46	-2.16837	-0.97769	-2.64996
C47	-3.05092	-1.05537	-3.72578
H48	-4.73648	-0.15861	-4.728
H49	-4.93161	1.712934	-3.10518
H50	-3.32921	1.882898	-1.20307
H51	-1.39749	-1.72659	-2.49819
H52	-2.95875	-1.87168	-4.4363
O53	0.704774	-1.56905	-0.23788
C54	1.482821	-2.41375	-0.75175
O55	2.615564	-2.26692	-1.25843
C56	0.896793	-3.84847	-0.76401
F57	1.795872	-4.76859	-1.1188
F58	0.411245	-4.17444	0.449734
F59	-0.13005	-3.9006	-1.6444
H60	3.302483	-1.14028	-1.14534
C61	0.340879	2.834677	-0.43693
H62	0.548062	3.584	-1.2105
H63	1.187684	2.843864	0.252201
O64	-0.88307	3.153562	0.139548
H65	-0.96858	2.554994	0.900562

Table S32. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_2OH^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	Y	z
Rh1	0.1815	0.76211	-0.52685
N2	-0.32059	-0.38531	1.205243
C3	3.247099	1.397078	-0.01751
O4	3.73154	0.210772	0.088755
C5	-1.51334	-0.68928	0.70742
O6	2.079349	1.757501	-0.17664
N7	-1.632	-0.15163	-0.51128
C8	4.34358	2.483945	0.079866
F9	3.815939	3.706109	-0.00712
F10	4.989844	2.375529	1.25209
F11	5.229592	2.321567	-0.91429
H12	0.159881	2.504377	-1.67025
C13	-4.65477	-2.79982	2.705209

C14	-4.2607	-3.19613	1.426093
C15	-3.23364	-2.52136	0.768402
C16	-2.58909	-1.44763	1.397216
C17	-2.97969	-1.05852	2.68659
C18	-4.0134	-1.73092	3.334016
H19	-5.4604	-3.32354	3.212183
H20	-4.7548	-4.0311	0.937898
H21	-2.92354	-2.83037	-0.22439
H22	-2.47605	-0.22847	3.172172
H23	-4.31766	-1.4201	4.3293
C24	1.597298	-1.76068	4.685741
C25	0.958645	-2.67213	3.842677
C26	0.321858	-2.23726	2.682811
C27	0.296616	-0.86795	2.368202
C28	0.950637	0.045307	3.210592
C29	1.596326	-0.40236	4.36056
H30	2.100484	-2.10744	5.583658
H31	0.969277	-3.73249	4.079617
H32	-0.14354	-2.94844	2.008679
H33	0.929737	1.1003	2.953096
H34	2.096356	0.313056	5.007681
C35	-4.78157	-0.28144	-3.29284
C36	-4.96086	0.379564	-2.07579
C37	-3.92397	0.439009	-1.14569
C38	-2.70137	-0.19064	-1.42244
C39	-2.5234	-0.85889	-2.64563
C40	-3.55993	-0.89632	-3.57594
H41	-5.59029	-0.31824	-4.01707
H42	-5.91055	0.857016	-1.85155
H43	-4.05168	0.958237	-0.20091
H44	-1.57765	-1.35712	-2.83587
H45	-3.41619	-1.41675	-4.51879
O46	-0.60905	2.347507	0.555501
C47	-0.51589	3.463047	-0.01864
O48	-0.08366	3.656819	-1.18434
C49	-0.95615	4.712313	0.770237
F50	-1.52766	4.384887	1.933643
F51	0.11654	5.479771	1.019294
F52	-1.83363	5.423059	0.046244
O53	0.80436	-0.97337	-1.55323

C54	1.429949	-1.92086	-0.96836
O55	2.342528	-1.85411	-0.13455
C56	0.903971	-3.326	-1.35499
F57	1.786146	-4.28984	-1.0873
F58	-0.22173	-3.57197	-0.63839
F59	0.580172	-3.38851	-2.65767
H60	3.052485	-0.582	0.028999
C61	0.337881	1.517206	-2.72072
H62	0.098029	2.455935	-3.23911
H63	-0.42438	0.797963	-3.03139
O64	1.640143	1.173644	-3.10344
H65	1.744586	0.237372	-2.87911

Table S33. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{ax})(CH_2OH^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.454766	0.382117	-0.04279
N2	-0.59329	-0.06839	1.778601
C3	3.310815	1.049819	-0.03177
O4	3.104725	1.289159	-1.24247
C5	-1.7109	-0.34634	1.086401
O6	2.423677	0.686694	0.797149
N7	-1.55926	0.00879	-0.18628
C8	4.730931	1.243374	0.536132
F9	5.179426	0.093666	1.051251
F10	5.58382	1.669332	-0.39438
F11	4.673658	2.161932	1.523449
H12	1.818066	1.919926	1.823633
C13	-5.21686	-2.05217	2.860352
C14	-4.80955	-2.47447	1.594041
C15	-3.67727	-1.9205	1.000125
C16	-2.93623	-0.94164	1.677895
C17	-3.3469	-0.52581	2.953893
C18	-4.48446	-1.07578	3.538414
H19	-6.10112	-2.48535	3.31958
H20	-5.37206	-3.24006	1.06763
H21	-3.35979	-2.25859	0.020286
H22	-2.77058	0.226726	3.481934
H23	-4.79708	-0.74543	4.524767
C24	0.890078	-2.19294	5.104295
C25	0.424353	-2.89152	3.988494

C26	-0.07916	-2.20748	2.884343
C27	-0.13515	-0.80291	2.893178
C28	0.34801	-0.1046	4.010737
C29	0.853803	-0.79712	5.108742
H30	1.287975	-2.73191	5.959416
H31	0.466282	-3.97718	3.969928
H32	-0.39448	-2.74756	1.998298
H33	0.313445	0.98131	4.00913
H34	1.220467	-0.24519	5.969937
C35	-4.31426	0.094059	-3.36067
C36	-4.39078	1.050169	-2.34638
C37	-3.4802	1.028843	-1.29017
C38	-2.49725	0.028602	-1.23549
C39	-2.4196	-0.93266	-2.25681
C40	-3.32629	-0.89287	-3.3142
H41	-5.02078	0.118494	-4.18518
H42	-5.15725	1.819413	-2.37861
H43	-3.5249	1.771024	-0.4985
H44	-1.66122	-1.7078	-2.19218
H45	-3.26575	-1.6399	-4.10043
O46	-0.00477	2.456484	0.333513
C47	0.418062	3.0956	1.292421
O48	1.382621	2.771219	2.107424
C49	-0.21828	4.454907	1.653146
F50	0.715227	5.415256	1.649172
F51	-1.17498	4.769937	0.781284
F52	-0.75439	4.377251	2.881387
O53	0.612993	-1.61358	-0.30052
C54	1.629706	-2.13961	-0.90646
O55	2.635113	-1.60849	-1.34625
C56	1.390398	-3.66239	-1.08804
F57	2.456437	-4.27285	-1.61261
F58	1.093386	-4.26239	0.082585
F59	0.341925	-3.85863	-1.92485
H60	1.923631	0.960251	-1.48229
C61	0.709616	0.759373	-2.28193
H62	0.115172	-0.13007	-2.50303
H63	1.565832	0.695515	-2.96881
O64	0.055919	1.969724	-2.57393
H65	-0.82999	1.936263	-2.18871

Rh(NN^F) complexes in TFAH

Table S34. [Rh^I(NN^F)(TFA)(TFAH)]$^-$

Atom	x	y	z
Rh1	0.272664	0.153208	0.007484
N2	-0.71667	-0.41	1.772591
C3	3.212526	0.548199	0.729521
O4	3.7627	-0.11495	-0.21962
C5	-1.76707	-0.91452	1.117821
O6	2.050751	0.954642	0.844906
N7	-1.56298	-0.7866	-0.19499
C8	1.556978	-0.07635	-2.71477
O9	0.649105	0.458874	-2.0449
O10	2.684292	-0.51493	-2.35612
C11	1.278385	-0.18975	-4.23492
F12	1.734007	-1.35179	-4.73778
F13	-0.03388	-0.10783	-4.51896
F14	1.899548	0.812257	-4.90278
C15	4.158533	0.89778	1.900193
F16	5.330257	0.245366	1.832869
F17	4.421969	2.221429	1.908857
F18	3.579869	0.586924	3.077291
H19	3.146259	-0.28814	-1.13397
C20	-5.28551	-2.59848	2.935517
C21	-4.62298	-3.29109	1.926176
C22	-3.48108	-2.74438	1.350243
C23	-2.97582	-1.5012	1.747436
C24	-3.66548	-0.82774	2.762269
C25	-4.80311	-1.36303	3.357117
F26	-6.3828	-3.11907	3.499102
F27	-5.07928	-4.48738	1.529154
F28	-2.85954	-3.45752	0.402035
F29	-3.25286	0.37531	3.181326
F30	-5.44769	-0.68961	4.320438
C31	0.528756	-0.99429	5.756339
C32	-0.0207	-2.05661	5.047437
C33	-0.44944	-1.87175	3.738087
C34	-0.38005	-0.62233	3.091869
C35	0.193064	0.428169	3.836413

C36	0.642226	0.248674	5.139286
F37	0.941952	-1.16458	7.023481
F38	-0.11496	-3.26685	5.624779
F39	-0.90832	-2.95026	3.073886
F40	0.301001	1.642129	3.292228
F41	1.165597	1.278606	5.822162
C42	-4.20123	-1.13673	-3.4587
C43	-4.62643	-0.49303	-2.30222
C44	-3.77103	-0.38583	-1.21165
C45	-2.47714	-0.93671	-1.21787
C46	-2.07607	-1.573	-2.4089
C47	-2.91619	-1.66976	-3.51093
F48	-5.025	-1.24836	-4.5136
F49	-5.85858	0.041016	-2.24925
F50	-4.20572	0.300468	-0.13767
F51	-0.86077	-2.12378	-2.49128
F52	-2.50772	-2.30043	-4.62102

Table S35. $Rh^{I}(NN^{F})(TFAH)_2$

Atom	x	y	z
Rh1	0.219292	0.351431	-0.14893
N2	-0.81141	-0.01816	1.593446
C3	3.171107	1.083195	0.200667
O4	3.524823	0.747031	-1.01957
C5	-1.83189	-0.61431	0.974096
O6	2.038538	1.09078	0.667289
N7	-1.69965	-0.45356	-0.34502
C8	0.281687	1.092082	-2.9556
O9	1.023402	0.482532	-2.17506
O10	-0.75108	1.786273	-2.58121
C11	0.481409	1.015959	-4.47859
F12	0.378426	2.231714	-5.0272
F13	1.681509	0.506423	-4.76086
F14	-0.46654	0.222495	-4.99886
C15	4.380299	1.478149	1.070841
F16	5.092639	2.439303	0.464725
F17	3.972379	1.921134	2.259182
F18	5.171259	0.407669	1.250775
H19	2.733051	0.506337	-1.55214
C20	-4.92559	-2.81984	2.979431

C21	-4.22192	-3.40664	1.929927
C22	-3.2228	-2.68473	1.285729
C23	-2.90739	-1.37424	1.659686
C24	-3.62695	-0.8113	2.71897
C25	-4.62799	-1.51792	3.376947
F26	-5.88244	-3.50443	3.603952
F27	-4.49974	-4.6585	1.557413
F28	-2.55098	-3.28302	0.295713
F29	-3.37105	0.440281	3.116285
F30	-5.308	-0.95438	4.378397
C31	0.63632	-0.78103	5.474357
C32	0.32335	-1.84817	4.636741
C33	-0.16762	-1.5983	3.36067
C34	-0.38391	-0.29293	2.890301
C35	-0.04222	0.761665	3.750013
C36	0.460387	0.525813	5.025755
F37	1.107741	-1.00995	6.702543
F38	0.510965	-3.10492	5.054753
F39	-0.41095	-2.6447	2.554484
F40	-0.19872	2.024007	3.34603
F41	0.764978	1.548727	5.830567
C42	-4.52214	-1.24678	-3.38244
C43	-4.93592	-0.65785	-2.19125
C44	-4.01124	-0.39253	-1.18703
C45	-2.65399	-0.74193	-1.30978
C46	-2.26928	-1.31266	-2.53351
C47	-3.1766	-1.56011	-3.55669
F48	-5.4054	-1.49973	-4.35213
F49	-6.21997	-0.32489	-2.02313
F50	-4.44261	0.246459	-0.08612
F51	-0.97664	-1.616	-2.74203
F52	-2.76241	-2.11012	-4.70229
H53	-0.78104	1.700042	-1.56214

Table S36. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})]_2(\mu^2\text{-}TFA^{eq})_2 \cdot 2TFAH$

Atom	x	y	z
Rh1	-1.81541	-0.81342	0.946389
N2	-2.98419	-0.45521	2.613864
C3	0.904302	0.5755	1.85675
O4	1.293618	1.368486	0.961557

C5	-4.08101	-0.93967	2.031512
O6	0.050186	-0.3364	1.832459
N7	-3.79889	-1.32866	0.795561
C8	1.601905	0.709111	3.243796
F9	2.577498	1.637108	3.22553
F10	0.713796	1.065391	4.190428
F11	2.149118	-0.4621	3.598734
C12	-7.92612	-1.20387	3.897015
C13	-7.40691	-2.30586	3.21931
C14	-6.16001	-2.21085	2.612899
C15	-5.40974	-1.03073	2.670678
C16	-5.9491	0.059898	3.363224
C17	-7.1979	-0.01719	3.969859
F18	-9.11927	-1.2856	4.477731
F19	-8.09801	-3.44416	3.163381
F20	-5.67756	-3.28782	1.986847
F21	-5.27355	1.209401	3.443027
F22	-7.70115	1.036352	4.612615
C23	-2.15539	-0.63539	6.733615
C24	-2.61663	-1.7708	6.070284
C25	-2.88893	-1.7016	4.711494
C26	-2.7257	-0.51298	3.982546
C27	-2.25733	0.612634	4.673635
C28	-1.97508	0.555901	6.034715
F29	-1.89941	-0.68682	8.040341
F30	-2.7955	-2.91254	6.738922
F31	-3.34057	-2.80368	4.090737
F32	-2.10337	1.769592	4.035523
F33	-1.55356	1.644729	6.679217
C34	-6.4427	-1.76173	-2.43223
C35	-6.35926	-0.53751	-1.77142
C36	-5.48805	-0.39634	-0.69814
C37	-4.69804	-1.46813	-0.25923
C38	-4.80995	-2.69203	-0.9302
C39	-5.66978	-2.84335	-2.01193
F40	-7.28286	-1.90514	-3.45632
F41	-7.11749	0.488337	-2.16622
F42	-5.43212	0.775022	-0.0551
F43	-4.11647	-3.74337	-0.49275
F44	-5.78735	-4.01997	-2.62766

O45	-2.38236	0.916291	0.055707
C46	-2.0433	2.097407	0.424648
O47	-1.38158	2.442465	1.397976
C48	-2.55835	3.159703	-0.58901
F49	-2.34103	4.398678	-0.13568
F50	-1.89801	3.021054	-1.76472
F51	-3.86745	3.014487	-0.83313
O52	-1.34049	-2.65259	1.896164
C53	-1.24084	-3.86848	1.744546
O54	-1.32812	-4.60065	0.688255
C55	-0.99193	-4.72481	3.015084
F56	-0.01009	-5.60637	2.805633
F57	-0.6604	-3.94332	4.047179
F58	-2.11468	-5.3939	3.322361
H59	-1.45705	-4.17732	-0.21488
Rh60	1.911554	0.770042	-0.97143
N61	3.115057	0.382354	-2.60375
C62	-0.8504	-0.55246	-1.90115
O63	-1.27324	-1.35207	-1.02691
C64	4.19583	0.89438	-2.00966
O65	0.045554	0.316652	-1.86355
N66	3.883059	1.281403	-0.78223
C67	-1.56895	-0.60093	-3.28217
F68	-2.55133	-1.5232	-3.30573
F69	-0.70315	-0.89487	-4.26719
F70	-2.11787	0.594616	-3.54613
C71	8.056074	1.237269	-3.83267
C72	7.517367	2.320492	-3.14035
C73	6.26525	2.200856	-2.54929
C74	5.530545	1.012005	-2.63095
C75	6.09085	-0.06004	-3.33621
C76	7.342799	0.043598	-3.93237
F77	9.252896	1.344148	-4.40176
F78	8.194072	3.465968	-3.05725
F79	5.763634	3.264314	-1.91501
F80	5.432622	-1.21728	-3.44029
F81	7.862642	-0.99189	-4.59111
C82	2.237827	0.539303	-6.71231
C83	2.722216	1.675508	-6.06742
C84	3.015926	1.618025	-4.7122

C85	2.856178	0.435965	-3.9714
C86	2.358588	-0.68898	-4.64258
C87	2.053466	-0.64284	-5.99872
F88	1.959691	0.581863	-8.01502
F89	2.900296	2.809988	-6.74943
F90	3.47436	2.725664	-4.10918
F91	2.190134	-1.83204	-3.98284
F92	1.602938	-1.7308	-6.62478
C93	6.436358	1.935153	2.477234
C94	6.437092	0.695334	1.840795
C95	5.589604	0.480392	0.760846
C96	4.746096	1.494613	0.288344
C97	4.763708	2.733406	0.941556
C98	5.598787	2.956802	2.030573
F99	7.255347	2.151349	3.50595
F100	7.250912	-0.27477	2.265106
F101	5.603999	-0.70751	0.145136
F102	4.000185	3.724941	0.483039
F103	5.634297	4.148366	2.627892
O104	2.441007	-0.9556	-0.05313
C105	2.04923	-2.13369	-0.3768
O106	1.369954	-2.49198	-1.33276
C107	2.55682	-3.21378	0.621999
F108	1.562498	-4.09266	0.881922
F109	2.966811	-2.70028	1.786437
F110	3.574654	-3.89859	0.074434
O111	1.50048	2.607067	-1.94916
C112	0.981031	3.708299	-1.78269
O113	0.725388	4.364554	-0.70178
C114	0.600504	4.495112	-3.06438
F115	-0.48384	5.247657	-2.87302
F116	0.372647	3.647286	-4.07298
F117	1.62889	5.293302	-3.40022
H118	1.057019	4.021028	0.186601
H119	0.478401	-3.39724	-2.38423
O120	-0.0397	-3.65826	-3.1965
C121	-1.24579	-4.07959	-2.92531
O122	-1.74576	-4.28128	-1.83218
C123	-2.06182	-4.36561	-4.21258
F124	-3.37027	-4.2341	-3.96531

F125	-1.72677	-3.5372	-5.2082
F126	-1.82906	-5.62852	-4.61381
H127	-0.64901	3.518012	2.401711
O128	-0.13185	3.874187	3.179413
C129	1.0886	4.206065	2.852674
O130	1.579231	4.259151	1.737041
C131	1.928575	4.576937	4.101043
F132	3.220915	4.676374	3.779592
F133	1.513671	5.759723	4.587556
F134	1.793814	3.654809	5.064595

Table S37. $[Rh^{III}(NN^{F})(TFA)_3(TFAH)^{eq}]^-$

Atom	x	y	z
Rh1	0.234151	0.185052	0.03765
N2	-0.76137	-0.38373	1.71274
C3	2.84852	1.289955	0.700795
O4	2.795686	2.17456	-0.13373
C5	-1.93006	-0.61685	1.114524
O6	2.045495	0.300266	0.934563
N7	-1.87749	-0.2031	-0.14564
C8	0.789591	1.116754	-2.9042
O9	1.10318	0.494466	-1.89323
O10	-0.12493	2.00995	-3.07081
C11	1.563138	0.818182	-4.21061
F12	0.7096	0.355084	-5.14735
F13	2.127552	1.943421	-4.68704
F14	2.516643	-0.08987	-4.02143
C15	4.024983	1.249486	1.719969
F16	4.827509	2.317295	1.584202
F17	3.56652	1.247182	2.995009
F18	4.783669	0.145215	1.563847
H19	-0.59199	2.342372	-2.18036
C20	-5.20387	-2.58255	3.080615
C21	-4.76578	-3.03434	1.838742
C22	-3.71177	-2.38583	1.202958
C23	-3.08054	-1.2796	1.780879
C24	-3.54012	-0.84587	3.027886
C25	-4.59078	-1.48462	3.678444
F26	-6.21289	-3.20205	3.698935
F27	-5.35099	-4.09429	1.270281
F28	-3.30615	-2.86041	0.022602

F29	-2.97895	0.209473	3.626805
F30	-5.01878	-1.04787	4.868485
C31	1.213008	-2.08451	5.002768
C32	0.431868	-2.8999	4.189563
C33	-0.24909	-2.35223	3.108247
C34	-0.19692	-0.97673	2.8336
C35	0.597531	-0.17615	3.67295
C36	1.300503	-0.71988	4.740624
F37	1.869698	-2.61129	6.043953
F38	0.34701	-4.21256	4.446791
F39	-0.96832	-3.17252	2.33144
F40	0.67689	1.132592	3.455234
F41	2.041784	0.062644	5.53244
C42	-4.96761	0.247784	-2.96794
C43	-5.18435	0.626279	-1.64742
C44	-4.16884	0.48384	-0.70893
C45	-2.92144	-0.07099	-1.04009
C46	-2.72692	-0.42164	-2.38663
C47	-3.72792	-0.26738	-3.33841
F48	-5.94385	0.379777	-3.87614
F49	-6.36855	1.140587	-1.2857
F50	-4.40302	0.912647	0.543967
F51	-1.54902	-0.92388	-2.77095
F52	-3.51533	-0.63105	-4.60857
O53	-0.13171	2.156888	0.655167
C54	-0.82731	3.014172	0.051485
O55	-1.24337	3.032444	-1.12691
C56	-1.22594	4.210767	0.958015
F57	-1.97291	5.111315	0.300582
F58	-1.94365	3.777196	2.01594
F59	-0.13627	4.841632	1.429194
O60	0.413982	-1.82112	-0.24122
C61	1.487867	-2.42245	-0.65535
O62	2.544846	-1.9936	-1.06923
C63	1.263828	-3.96237	-0.55037
F64	2.324291	-4.64885	-1.00402
F65	1.059897	-4.33674	0.735917
F66	0.186189	-4.36504	-1.26005

Table S38. [$Rh^{III}(NN^{F})(TFA)_3(TFAH)^{ax}$]⁻

Atom	x	y	z
Rh1	0.305748	0.180603	0.034294
N2	-0.72188	-0.40843	1.704888
C3	2.840896	1.380952	0.829275
O4	2.72303	2.349218	0.100205
C5	-1.87019	-0.65289	1.075253
O6	2.105889	0.321784	0.951424
N7	-1.79304	-0.25423	-0.18888
C8	0.53885	1.020506	-2.83898
O9	1.150094	0.52951	-1.86725
O10	-0.51272	1.719052	-2.85939
C11	1.12711	0.716086	-4.24013
F12	2.302419	0.087135	-4.18058
F13	0.265234	-0.06316	-4.92849
F14	1.294488	1.856451	-4.94023
C15	4.018671	1.309932	1.845664
F16	4.772328	2.420605	1.801074
F17	3.5561	1.186449	3.114166
F18	4.826702	0.257766	1.608103
H19	-0.84075	2.431498	-1.81776
C20	-5.22154	-2.55817	2.969774
C21	-4.74256	-3.04233	1.755755
C22	-3.6644	-2.4132	1.141193
C23	-3.04671	-1.29738	1.715864
C24	-3.54863	-0.83041	2.934368
C25	-4.62536	-1.44821	3.561966
F26	-6.25444	-3.15824	3.566983
F27	-5.3123	-4.11377	1.193559
F28	-3.2207	-2.91564	-0.01354
F29	-3.00294	0.237236	3.526385
F30	-5.09407	-0.98006	4.724301
C31	1.176142	-2.13691	5.025003
C32	0.416058	-2.9449	4.185376
C33	-0.24167	-2.38688	3.094851
C34	-0.18615	-1.00888	2.834037
C35	0.588241	-0.21728	3.699495
C36	1.267016	-0.76978	4.777934
F37	1.809953	-2.67272	6.075916
F38	0.329265	-4.26057	4.425579

F39	-0.93838	-3.20092	2.290489
F40	0.672835	1.094706	3.493885
F41	1.988372	0.006399	5.594125
C42	-4.92111	0.21378	-2.96635
C43	-5.07163	0.697421	-1.67131
C44	-4.03936	0.542604	-0.75373
C45	-2.84471	-0.11961	-1.08073
C46	-2.71602	-0.58109	-2.40123
C47	-3.73527	-0.41728	-3.33257
F48	-5.91279	0.353633	-3.85603
F49	-6.20452	1.320545	-1.31586
F50	-4.1992	1.061102	0.477578
F51	-1.59715	-1.20077	-2.78066
F52	-3.59403	-0.88305	-4.57867
O53	-0.11901	2.168607	0.662316
C54	-0.71097	3.106529	0.114773
O55	-1.14516	3.21783	-1.07977
C56	-1.02093	4.349277	0.984001
F57	-2.35675	4.521814	1.065777
F58	-0.53952	4.224355	2.222836
F59	-0.49489	5.454765	0.430505
O60	0.537956	-1.80403	-0.227
C61	1.631559	-2.37986	-0.63511
O62	2.676018	-1.92874	-1.05086
C63	1.441788	-3.92306	-0.51068
F64	2.526316	-4.58751	-0.93755
F65	1.226646	-4.28362	0.777807
F66	0.386034	-4.36097	-1.23104

Table S39. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})(TFAH^{eq})$

Atom	x	y	z
Rh1	0.086085	0.384395	-0.38278
N2	-0.70391	0.060705	1.465475
C3	3.067789	0.842751	-0.50229
O4	3.286188	0.031573	-1.42683
C5	-1.89656	-0.3192	0.994374
O6	1.996309	1.063968	0.132381
N7	-1.88358	-0.20588	-0.32782
C8	0.937485	1.089247	-3.3745
O9	0.441123	0.3592	-2.50264

O10	1.364619	2.286689	-3.27115
C11	1.09738	0.464989	-4.78374
F12	1.082623	1.401904	-5.73512
F13	2.267018	-0.19124	-4.8368
F14	0.106577	-0.40466	-5.01695
C15	4.279345	1.715491	-0.0768
F16	4.695439	2.444545	-1.12473
F17	3.977067	2.545809	0.926407
F18	5.290404	0.922518	0.317268
H19	1.206261	2.746711	-2.31574
C20	-5.17333	-1.70721	3.377326
C21	-4.80593	-2.40347	2.227023
C22	-3.73931	-1.94731	1.461367
C23	-3.02687	-0.79518	1.816033
C24	-3.41372	-0.11496	2.976916
C25	-4.47643	-0.56065	3.755413
F26	-6.19061	-2.13906	4.116487
F27	-5.46829	-3.5049	1.872324
F28	-3.39661	-2.64654	0.375345
F29	-2.77043	0.992534	3.356168
F30	-4.83341	0.105094	4.853769
C31	1.345317	-1.00266	4.972583
C32	0.602948	-1.96844	4.296328
C33	-0.08481	-1.62103	3.140138
C34	-0.07713	-0.30525	2.649173
C35	0.682255	0.648122	3.347057
C36	1.390817	0.305463	4.49352
F37	2.012225	-1.33103	6.078259
F38	0.567941	-3.22392	4.750459
F39	-0.76263	-2.57376	2.484784
F40	0.733187	1.902697	2.906902
F41	2.103944	1.224536	5.146027
C42	-4.96184	-0.07201	-3.18215
C43	-5.10856	0.622428	-1.98375
C44	-4.09641	0.577686	-1.0314
C45	-2.93392	-0.18164	-1.23355
C46	-2.81129	-0.87098	-2.44963
C47	-3.80636	-0.81483	-3.41842
F48	-5.92578	-0.02717	-4.1016
F49	-6.21143	1.340543	-1.75881

F50	-4.24402	1.281464	0.099104
F51	-1.71648	-1.59853	-2.68866
F52	-3.66917	-1.48091	-4.56635
O53	-0.58359	2.295673	-0.10914
C54	0.054742	3.360058	-0.38804
O55	0.96206	3.551002	-1.21406
C56	-0.41653	4.567414	0.46899
F57	0.168871	5.701176	0.077635
F58	-1.74912	4.718429	0.369614
F59	-0.1112	4.349979	1.759497
O60	0.455293	-1.68654	-0.40273
C61	1.119603	-2.3876	-1.18766
O62	2.117847	-2.06114	-1.90749
C63	0.726243	-3.88313	-1.27685
F64	1.486267	-4.58554	-0.41837
F65	-0.55806	-4.05242	-0.94909
F66	0.925205	-4.35213	-2.51138
H67	2.527411	-1.08267	-1.70961

Table S40. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})_2$

Atom	x	y	z
Rh1	0.128596	0.218709	-0.4946
N2	-0.6014	-0.13409	1.392994
C3	3.119938	0.754262	-0.67402
O4	3.375336	-0.08603	-1.5575
C5	-1.81287	-0.47283	0.96127
O6	2.031722	0.982381	-0.06583
N7	-1.82287	-0.426	-0.37037
C8	1.005187	1.214851	-3.22092
O9	0.419622	0.301707	-2.56361
O10	1.406839	2.332144	-2.84655
C11	1.244124	0.823208	-4.70472
F12	1.850138	1.799583	-5.38255
F13	2.009862	-0.28036	-4.76426
F14	0.069044	0.553701	-5.30303
C15	4.269662	1.694729	-0.22109
F16	5.408489	1.428497	-0.86283
F17	3.930425	2.973619	-0.45926
F18	4.48133	1.553817	1.100643
H19	1.131794	2.981333	-1.65011

C20	-5.151	-1.48253	3.44689
C21	-4.80819	-2.30799	2.376872
C22	-3.72223	-1.97477	1.574722
C23	-2.96157	-0.82672	1.820861
C24	-3.32502	-0.01428	2.901211
C25	-4.4094	-0.33197	3.711468
F26	-6.18926	-1.79363	4.217454
F27	-5.51541	-3.41158	2.132638
F28	-3.4076	-2.78543	0.559931
F29	-2.63843	1.10088	3.167893
F30	-4.74621	0.459906	4.729926
C31	1.304591	-0.72749	5.086942
C32	0.557869	-1.76149	4.52642
C33	-0.07809	-1.56777	3.3059
C34	-0.01435	-0.33826	2.632087
C35	0.748428	0.684617	3.216378
C36	1.407001	0.495634	4.425915
F37	1.920468	-0.90782	6.255046
F38	0.467697	-2.9371	5.153545
F39	-0.76172	-2.58636	2.765868
F40	0.849905	1.867402	2.604409
F41	2.122523	1.48299	4.966529
C42	-4.95665	-0.10634	-3.14694
C43	-5.00713	0.64083	-1.97207
C44	-3.97866	0.533883	-1.0432
C45	-2.89718	-0.33785	-1.24368
C46	-2.86784	-1.07381	-2.43894
C47	-3.88041	-0.96017	-3.38442
F48	-5.93679	-0.00373	-4.04406
F49	-6.03169	1.468144	-1.74958
F50	-4.02664	1.293435	0.060272
F51	-1.84707	-1.89898	-2.68065
F52	-3.83617	-1.6729	-4.51092
O53	-0.65549	2.114635	-0.13921
C54	-0.11084	3.235498	-0.1429
O55	0.855696	3.65085	-0.85658
C56	-0.7189	4.299216	0.805855
F57	0.242823	5.065414	1.326866
F58	-1.56381	5.077765	0.108006
F59	-1.39574	3.715074	1.798195

O60	0.540901	-1.81418	-0.58074
C61	1.191699	-2.47966	-1.41125
O62	2.168275	-2.12339	-2.14051
C63	0.755782	-3.95322	-1.60876
F64	1.82482	-4.75418	-1.67976
F65	-0.02361	-4.36039	-0.60369
F66	0.067641	-4.04709	-2.75692
H67	2.587999	-1.15528	-1.90843

Table S41. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{eq})_2$

Atom	x	y	z
Rh1	0.137267	0.246372	-0.35811
N2	-0.6947	-0.04929	1.473396
C3	3.107564	1.103906	-0.47996
O4	3.509531	0.328935	-1.41491
C5	-1.88507	-0.39523	0.974877
O6	2.062759	1.019336	0.18528
N7	-1.82144	-0.30734	-0.35015
C8	0.587335	0.904241	-3.46341
O9	0.555578	0.158889	-2.47482
O10	0.739969	2.172735	-3.50725
C11	0.355306	0.238012	-4.84304
F12	0.896058	0.950769	-5.83254
F13	0.86228	-0.99539	-4.86308
F14	-0.977	0.159872	-5.0492
C15	4.082875	2.262922	-0.15799
F16	4.44854	2.879775	-1.28814
F17	3.514663	3.148634	0.660011
F18	5.180787	1.765318	0.435946
H19	0.844991	2.63344	-2.5473
C20	-5.3161	-1.54845	3.262581
C21	-4.98268	-2.25369	2.107231
C22	-3.86385	-1.87816	1.372579
C23	-3.06275	-0.79785	1.765124
C24	-3.41805	-0.10684	2.931171
C25	-4.53262	-0.47281	3.677423
F26	-6.38398	-1.90293	3.970408
F27	-5.72952	-3.28664	1.717
F28	-3.56142	-2.58361	0.279028
F29	-2.69573	0.936463	3.347237

F30	-4.85735	0.203918	4.778971
C31	1.273874	-1.31202	4.959041
C32	0.491527	-2.22123	4.249352
C33	-0.16863	-1.80956	3.097599
C34	-0.09571	-0.47985	2.650032
C35	0.701146	0.416168	3.380274
C36	1.382275	0.007422	4.521534
F37	1.915275	-1.70387	6.059285
F38	0.394632	-3.48602	4.666219
F39	-0.88908	-2.70633	2.41323
F40	0.814757	1.679688	2.9745
F41	2.131633	0.873371	5.206573
C42	-4.76974	0.229125	-3.29104
C43	-4.89071	0.894551	-2.07259
C44	-3.92209	0.71953	-1.09099
C45	-2.83595	-0.14866	-1.284
C46	-2.73788	-0.80683	-2.51939
C47	-3.68589	-0.61746	-3.51804
F48	-5.69084	0.402266	-4.23819
F49	-5.9245	1.711871	-1.85807
F50	-4.03759	1.399976	0.057061
F51	-1.70877	-1.62358	-2.74724
F52	-3.56906	-1.24933	-4.68612
O53	-0.52714	2.199041	-0.12012
C54	0.121519	3.236455	-0.45094
O55	0.938833	3.389683	-1.38074
C56	-0.12754	4.453394	0.479254
F57	0.066249	5.60698	-0.16932
F58	-1.37309	4.447399	0.974644
F59	0.738829	4.391358	1.507884
O60	0.538963	-1.76622	-0.29971
C61	1.497641	-2.36348	-0.88089
O62	2.493473	-1.90547	-1.46442
C63	1.338587	-3.90753	-0.81287
F64	2.417913	-4.53374	-1.28628
F65	1.145007	-4.29567	0.461555
F66	0.270765	-4.28881	-1.53499
H67	2.960417	-0.59003	-1.46833

Table S42. $[Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})(CH_3^{ax})]^-$

Atom	x	y	z
Rh1	0.422727	0.189251	0.128493
N2	-0.50659	-0.63108	1.832825
C3	3.001237	1.566545	0.891614
O4	2.722898	2.709121	0.480947
C5	-1.69251	-0.7181	1.23779
O6	2.347788	0.4891	0.865017
N7	-1.58714	-0.40169	-0.05133
C8	1.747163	1.056113	-2.43368
O9	0.674403	1.057913	-1.71729
O10	2.830715	0.524288	-2.25197
C11	1.519803	1.903243	-3.72085
F12	2.613048	1.93285	-4.50221
F13	0.505794	1.40426	-4.46771
F14	1.202336	3.182655	-3.42013
C15	4.359448	1.409282	1.62802
F16	5.181788	2.447439	1.408366
F17	4.143293	1.336932	2.964297
F18	5.005749	0.288041	1.262969
H19	1.474149	3.27168	-0.0059
C20	-5.38546	-1.73749	3.189653
C21	-4.98835	-2.42781	2.047873
C22	-3.78978	-2.09381	1.425628
C23	-2.96623	-1.07864	1.919015
C24	-3.38929	-0.4003	3.066239
C25	-4.58437	-0.72117	3.702531
F26	-6.5355	-2.0516	3.794171
F27	-5.75584	-3.41179	1.562795
F28	-3.43307	-2.7841	0.336352
F29	-2.65366	0.591193	3.577505
F30	-4.97284	-0.05337	4.795512
C31	0.719215	-2.01931	5.612607
C32	-0.076	-2.82795	4.808416
C33	-0.48812	-2.37208	3.561526
C34	-0.15367	-1.09289	3.085849
C35	0.665536	-0.30562	3.915446
C36	1.096853	-0.75859	5.157402
F37	1.117218	-2.44991	6.818718
F38	-0.42825	-4.05256	5.230163

F39	-1.21166	-3.20611	2.791272
F40	1.025032	0.917518	3.523459
F41	1.856856	0.022547	5.935566
C42	-4.56137	0.83584	-2.76246
C43	-4.57079	1.333186	-1.46459
C44	-3.60384	0.917148	-0.55664
C45	-2.61438	-0.01861	-0.90072
C46	-2.62453	-0.49156	-2.22384
C47	-3.58025	-0.0754	-3.14299
F48	-5.49376	1.228354	-3.64196
F49	-5.50347	2.223799	-1.09764
F50	-3.62357	1.457818	0.671275
F51	-1.70849	-1.37952	-2.62046
F52	-3.57885	-0.5637	-4.39085
O53	-0.66902	2.288855	0.665402
C54	-0.46542	3.358968	0.104642
O55	0.656579	3.872609	-0.2742
C56	-1.69094	4.24603	-0.2222
F57	-1.35614	5.483893	-0.61154
F58	-2.40762	3.678537	-1.21699
F59	-2.49167	4.348461	0.85318
C60	1.07676	-1.63594	-0.49243
H61	2.118483	-1.49684	-0.78002
H62	0.975029	-2.35418	0.326809
H63	0.463616	-1.93446	-1.34453

Table S43. $Rh^{III}(NN^{F})(TFA)(TFAH^{eq})_2(CH_3{}^{ax})$

Atom	x	y	z
Rh1	0.292255	0.085867	-0.40037
N2	-0.49744	-0.45113	1.400849
C3	3.22285	1.119989	0.748406
O4	3.266263	2.405972	0.879059
C5	-1.72624	-0.6135	0.921238
O6	2.406711	0.428469	0.144716
N7	-1.67697	-0.46771	-0.40604
C8	1.069186	1.480414	-3.08371
O9	0.674419	0.48396	-2.47033
O10	1.401223	2.643066	-2.64539
C11	1.204658	1.379321	-4.62348
F12	0.391149	2.273864	-5.20717

F13	2.467646	1.646295	-4.98852
F14	0.88036	0.159153	-5.05361
C15	4.360707	0.407617	1.517995
F16	3.972878	0.260999	2.802296
F17	4.587265	-0.80411	1.003783
F18	5.494333	1.112067	1.493293
H19	1.290079	2.839889	-1.6191
C20	-5.23275	-1.43992	3.244207
C21	-4.949	-2.20793	2.11647
C22	-3.81064	-1.93055	1.367726
C23	-2.93773	-0.89618	1.720955
C24	-3.24836	-0.13539	2.854479
C25	-4.38141	-0.40069	3.616001
F26	-6.31896	-1.69959	3.967433
F27	-5.76194	-3.20597	1.766179
F28	-3.55563	-2.68942	0.296786
F29	-2.46029	0.878689	3.224556
F30	-4.66079	0.338001	4.69091
C31	1.094914	-1.32223	5.194612
C32	0.281551	-2.25541	4.556175
C33	-0.24762	-1.96882	3.302961
C34	-0.01179	-0.74043	2.666979
C35	0.814225	0.175215	3.33256
C36	1.370679	-0.10582	4.573934
F37	1.611625	-1.59406	6.393721
F38	0.027975	-3.43023	5.138628
F39	-0.98988	-2.90313	2.688137
F40	1.088953	1.359017	2.759424
F41	2.156216	0.787436	5.176796
C42	-4.7215	0.523398	-3.13471
C43	-4.69935	1.138784	-1.88588
C44	-3.69996	0.817566	-0.97348
C45	-2.71985	-0.14494	-1.26678
C46	-2.76168	-0.74139	-2.53688
C47	-3.74431	-0.41388	-3.46386
F48	-5.67529	0.831174	-4.01456
F49	-5.62811	2.047106	-1.57328
F50	-3.6861	1.455582	0.203378
F51	-1.83895	-1.64708	-2.86953
F52	-3.76641	-1.00304	-4.66201

O53	-0.6659	2.207122	0.083054
C54	0.095508	3.146047	0.326501
O55	1.212148	3.395909	-0.26196
C56	-0.28325	4.137418	1.455045
F57	-0.54358	5.353989	0.946544
F58	-1.35852	3.722384	2.133374
F59	0.745169	4.251713	2.318103
C60	0.846162	-1.84854	-0.7529
H61	1.91577	-1.90953	-0.5422
H62	0.278786	-2.52123	-0.10726
H63	0.627375	-2.04314	-1.80376
H64	2.462166	2.865831	0.448215

Table S44. $Rh^{III}(NN^{F})(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.553888	-0.24517	-0.33957
N2	-0.34008	-0.58651	1.452632
C3	3.186917	0.883085	0.523312
O4	3.002287	1.988556	-0.06623
C5	-1.57837	-0.6268	0.96173
O6	2.564324	-0.18796	0.347953
N7	-1.51043	-0.50178	-0.36424
C8	1.524573	1.03994	-2.99245
O9	0.973488	0.096476	-2.4213
O10	2.256426	1.980207	-2.49686
C11	1.309511	1.200761	-4.51607
F12	0.391038	2.163203	-4.71974
F13	2.444656	1.557308	-5.12646
F14	0.864436	0.063395	-5.05296
C15	4.332904	0.835899	1.566054
F16	4.484285	2.027203	2.158126
F17	4.091777	-0.08242	2.515245
F18	5.485362	0.513646	0.952604
H19	2.459476	1.909497	-1.48816
C20	-5.15772	-1.0807	3.284424
C21	-4.95534	-1.87187	2.155026
C22	-3.7923	-1.71718	1.408022
C23	-2.81273	-0.78376	1.764254
C24	-3.04174	-0.00247	2.902516
C25	-4.19793	-0.14304	3.661634

F26	-6.26771	-1.22199	4.004567
F27	-5.87048	-2.77581	1.801301
F28	-3.62148	-2.49876	0.336808
F29	-2.1461	0.91448	3.283142
F30	-4.39563	0.618381	4.739072
C31	1.199902	-1.61456	5.224022
C32	0.303666	-2.47353	4.591609
C33	-0.21508	-2.13546	3.346788
C34	0.1177	-0.92837	2.716533
C35	1.022574	-0.08652	3.376133
C36	1.568053	-0.41885	4.609055
F37	1.704916	-1.93562	6.416102
F38	-0.04056	-3.62607	5.172649
F39	-1.04107	-2.99812	2.733431
F40	1.370928	1.079939	2.806593
F41	2.423764	0.405959	5.214368
C42	-4.42469	0.811039	-3.10145
C43	-4.33917	1.418119	-1.85148
C44	-3.38688	0.983716	-0.93658
C45	-2.51627	-0.07974	-1.22471
C46	-2.61946	-0.66476	-2.49605
C47	-3.55685	-0.22972	-3.42608
F48	-5.33461	1.224753	-3.98537
F49	-5.16138	2.424679	-1.54039
F50	-3.30973	1.612661	0.245723
F51	-1.80058	-1.66702	-2.82787
F52	-3.63983	-0.81354	-4.62448
O53	-0.13661	2.13133	-0.15566
C54	0.033094	3.139424	0.511232
O55	1.167693	3.634386	0.93178
C56	-1.19408	3.967496	0.962251
F57	-0.85229	5.169225	1.433274
F58	-2.03034	4.131046	-0.07198
F59	-1.83882	3.294284	1.931717
C60	0.807502	-2.24485	-0.62131
H61	1.869414	-2.44831	-0.47281
H62	0.196118	-2.79842	0.093367
H63	0.488606	-2.44512	-1.64528
H64	1.925565	3.060793	0.621153

Table S45. $[Rh^{IV}(NN^{F})(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax})]^{+}$

Atom	x	y	z
Rh1	0.333823	0.232272	-0.28282
N2	-0.41821	-0.42448	1.490786
C3	3.374821	0.445751	-0.03772
O4	3.68298	-0.11504	-1.0904
C5	-1.68181	-0.57911	1.041356
O6	2.219997	0.895893	0.311269
N7	-1.64132	-0.30427	-0.27664
C8	1.226711	0.545064	-3.2493
O9	0.492612	0.833844	-2.28928
O10	2.399563	0.03434	-3.23702
C11	0.689747	0.843735	-4.67275
F12	0.942004	-0.18543	-5.4812
F13	-0.63373	1.052051	-4.62992
F14	1.286735	1.941626	-5.14649
C15	4.431908	0.612956	1.083574
F16	5.647234	0.277368	0.677825
F17	4.439179	1.88013	1.526123
F18	4.076422	-0.19083	2.114137
H19	1.854019	2.493711	0.874568
C20	-5.09033	-1.58176	3.417516
C21	-4.90345	-2.20154	2.179618
C22	-3.7918	-1.87568	1.413496
C23	-2.84734	-0.93886	1.855375
C24	-3.05971	-0.3328	3.102757
C25	-4.16568	-0.64477	3.882902
F26	-6.1469	-1.88467	4.152035
F27	-5.78082	-3.09796	1.744565
F28	-3.62128	-2.48472	0.233937
F29	-2.19745	0.584735	3.554248
F30	-4.34883	-0.04986	5.055582
C31	1.45455	-1.95207	4.911028
C32	0.511003	-2.73795	4.236969
C33	-0.13214	-2.22801	3.121087
C34	0.140449	-0.92308	2.647092
C35	1.104199	-0.15899	3.342709
C36	1.750061	-0.65948	4.462696
F37	2.066911	-2.43434	5.975178
F38	0.258348	-3.97182	4.653301

F39	-0.97455	-3.01281	2.444011
F40	1.352589	1.088358	2.955667
F41	2.631425	0.080516	5.118985
C42	-4.54317	0.49352	-3.18194
C43	-4.76112	0.933031	-1.86965
C44	-3.82729	0.650982	-0.88642
C45	-2.65096	-0.07771	-1.18105
C46	-2.45543	-0.49637	-2.5192
C47	-3.38599	-0.22417	-3.50673
F48	-5.43422	0.759084	-4.11662
F49	-5.84971	1.633481	-1.58194
F50	-4.01895	1.130815	0.342023
F51	-1.37868	-1.21527	-2.82733
F52	-3.19687	-0.64803	-4.74773
O53	-0.43456	2.418803	0.146021
C54	0.174266	3.357311	0.650105
O55	1.420539	3.372684	1.035859
C56	-0.52357	4.724028	0.859252
F57	-0.13816	5.558857	-0.11515
F58	-1.84869	4.570186	0.804044
F59	-0.19029	5.245297	2.04218
C60	0.94634	-1.70574	-0.60057
H61	1.859645	-1.86842	-0.02651
H62	0.16006	-2.38735	-0.27268
H63	1.132854	-1.83031	-1.66731
H64	2.848975	-0.06012	-2.29798

Table S46. $Rh^{IV}(NN^{F})(TFA)_2(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.401736	0.371238	-0.25306
N2	-0.3363	-0.24527	1.501653
C3	3.454082	0.353188	-0.10145
O4	3.739975	-0.00598	-1.26004
C5	-1.60201	-0.38816	1.071383
O6	2.341475	0.678416	0.400363
N7	-1.58959	-0.08142	-0.23096
C8	1.221789	0.570507	-3.27382
O9	0.52575	0.901611	-2.30235
O10	2.394178	0.069401	-3.28958
C11	0.617572	0.781317	-4.68413

F12	0.719116	-0.3482	-5.39773
F13	-0.67541	1.122138	-4.60475
F14	1.279395	1.756088	-5.32221
C15	4.604285	0.408654	0.939774
F16	5.73651	-0.1078	0.4579
F17	4.833296	1.674563	1.317775
F18	4.251189	-0.30015	2.03627
C20	-4.9619	-1.64107	3.410458
C21	-4.73266	-2.20801	2.157425
C22	-3.63447	-1.79706	1.413656
C23	-2.75072	-0.81752	1.885379
C24	-2.99607	-0.27186	3.153441
C25	-4.09097	-0.676	3.911545
F25	-6.00735	-2.03089	4.132049
F26	-5.55591	-3.14506	1.686694
F27	-3.42205	-2.37598	0.223877
F28	-2.18107	0.644272	3.670466
F29	-4.30792	-0.1427	5.112886
C31	1.580672	-1.63866	4.95571
C32	0.702592	-2.48118	4.272547
C33	0.049464	-2.01545	3.141245
C34	0.244741	-0.70334	2.671756
C35	1.141808	0.124707	3.371946
C36	1.802671	-0.33803	4.50442
F36	2.205966	-2.08034	6.042095
F37	0.510049	-3.73083	4.697002
F38	-0.74945	-2.8522	2.464986
F39	1.3351	1.373327	2.974564
F40	2.632908	0.458533	5.172706
C42	-4.60697	0.591219	-3.06907
C43	-4.78648	1.053102	-1.76629
C44	-3.81109	0.820175	-0.80376
C45	-2.63427	0.1124	-1.11734
C46	-2.48552	-0.34726	-2.44015
C47	-3.45128	-0.11259	-3.40679
F47	-5.54265	0.811457	-3.98702
F48	-5.89359	1.723789	-1.44748
F49	-4.00745	1.297081	0.423959
F50	-1.41317	-1.06944	-2.77259
F51	-3.29137	-0.57373	-4.64596

O53	0.155503	2.493219	0.037901
C54	-0.69812	3.022077	0.836578
O55	-1.59027	2.471091	1.482907
C56	-0.50948	4.560771	0.959001
F57	-1.44504	5.116598	1.742889
F58	0.697755	4.851327	1.484994
F59	-0.58253	5.149051	-0.25308
C60	0.860436	-1.63325	-0.59421
H61	1.731774	-1.88511	0.013735
H62	0.014244	-2.26506	-0.31969
H63	1.091773	-1.75403	-1.65348
H64	2.90438	0.031207	-2.32904

Table S47. $Rh^{IV}(NN^{F})(TFA)_2(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.433356	0.147835	-0.17672
N2	-0.30999	-0.60039	1.582509
C3	3.093303	1.47328	0.088646
O4	2.764136	2.55218	-0.41532
C5	-1.58174	-0.64449	1.148016
O6	2.396501	0.431014	0.331559
N7	-1.56703	-0.31327	-0.14583
C8	1.336835	0.684625	-2.99038
O9	0.443399	0.857189	-2.05236
O10	2.415334	0.130769	-2.92973
C11	0.816412	1.298404	-4.32006
F12	1.667046	1.07982	-5.32457
F13	-0.37677	0.752281	-4.65273
F14	0.636445	2.627733	-4.19515
C15	4.563237	1.294722	0.557534
F16	5.306075	2.365787	0.269154
F17	4.587235	1.111074	1.895611
F18	5.121052	0.218269	-0.01874
H19	1.44839	3.223556	-0.62509
C20	-5.08001	-1.5248	3.454152
C21	-4.88891	-2.14048	2.217589
C22	-3.74377	-1.8583	1.482131
C23	-2.77509	-0.96438	1.953297
C24	-2.99154	-0.35937	3.197108
C25	-4.12884	-0.63335	3.948214

F26	-6.1713	-1.79003	4.164276
F27	-5.79632	-2.99826	1.752135
F28	-3.57465	-2.47145	0.304991
F29	-2.1064	0.516563	3.682019
F30	-4.31697	-0.04143	5.127016
C31	1.479936	-2.10721	5.061838
C32	0.510828	-2.87021	4.409879
C33	-0.10121	-2.37367	3.267519
C34	0.224695	-1.10546	2.753239
C35	1.214166	-0.36153	3.424505
C36	1.834009	-0.85216	4.566913
F37	2.065141	-2.57855	6.15857
F38	0.187792	-4.07679	4.87733
F39	-0.99569	-3.14081	2.629738
F40	1.534372	0.851078	2.985185
F41	2.749758	-0.12483	5.203052
C42	-4.43344	1.072281	-2.8649
C43	-4.52289	1.470974	-1.53149
C44	-3.60462	0.995592	-0.60571
C45	-2.58886	0.099289	-0.9825
C46	-2.51843	-0.28088	-2.33725
C47	-3.42592	0.196832	-3.271
F48	-5.31351	1.527593	-3.75101
F49	-5.47715	2.3228	-1.15565
F50	-3.67233	1.442953	0.652746
F51	-1.57943	-1.13752	-2.72897
F52	-3.35198	-0.18684	-4.54323
O53	-0.52362	2.253525	0.43801
C54	-0.40801	3.352777	-0.10079
O55	0.626056	3.848652	-0.68935
C56	-1.64662	4.27983	-0.13375
F57	-1.32981	5.553529	-0.36754
F58	-2.47226	3.857895	-1.11911
F59	-2.31242	4.203377	1.026034
C60	1.048649	-1.75298	-0.66353
H61	1.682467	-2.08601	0.158763
H62	0.163551	-2.37691	-0.78859
H63	1.623318	-1.63637	-1.58033

Table S48. $Rh^{II}(NN^{F})(TFA)(TFAH)$

Atom	x	y	z
Rh1	0.200707	0.256014	-0.0101
N2	-0.75356	-0.30125	1.743747
C3	3.113445	0.474632	0.771957
O4	3.561947	-0.36015	-0.08394
C5	-1.79885	-0.83399	1.10332
O6	2.000166	1.026848	0.805263
N7	-1.61875	-0.66792	-0.20847
C8	1.436625	0.010202	-2.65254
O9	0.59625	0.705778	-2.01407
O10	2.378141	-0.68228	-2.20432
C11	1.245767	0.041628	-4.191
F12	1.975948	-0.89633	-4.79916
F13	-0.04855	-0.15822	-4.50687
F14	1.610087	1.245073	-4.67043
C15	4.06138	0.788716	1.95263
F16	5.280914	0.283926	1.767207
F17	4.156172	2.110877	2.131461
F18	3.536585	0.243095	3.070125
H19	2.946131	-0.50044	-0.96982
C20	-5.19333	-2.67518	2.966471
C21	-4.50837	-3.34861	1.955903
C22	-3.40558	-2.74824	1.358354
C23	-2.96698	-1.47795	1.74588
C24	-3.66948	-0.82504	2.764534
C25	-4.77446	-1.40965	3.373464
F26	-6.24881	-3.2422	3.54442
F27	-4.90518	-4.56404	1.576247
F28	-2.75312	-3.42128	0.403909
F29	-3.29357	0.394036	3.165965
F30	-5.43602	-0.76474	4.335383
C31	0.667366	-0.97678	5.645291
C32	0.165366	-2.0465	4.907286
C33	-0.31398	-1.83192	3.619816
C34	-0.34491	-0.54897	3.049204
C35	0.184215	0.506521	3.808652
C36	0.68307	0.301951	5.090166
F37	1.132997	-1.176	6.879055
F38	0.167431	-3.27738	5.427577

F39	-0.73234	-2.89123	2.907698
F40	0.207822	1.737564	3.293117
F41	1.169323	1.324893	5.796069
C42	-4.16138	-1.32259	-3.48844
C43	-4.65726	-0.66397	-2.36558
C44	-3.82823	-0.44079	-1.27139
C45	-2.50295	-0.8967	-1.25486
C46	-2.0276	-1.54682	-2.40336
C47	-2.83723	-1.75847	-3.51125
F48	-4.95266	-1.53666	-4.53997
F49	-5.92234	-0.23527	-2.34752
F50	-4.31517	0.236379	-0.22004
F51	-0.76457	-1.99098	-2.42639
F52	-2.36333	-2.3916	-4.58459

Table S49. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.588563	0.429642	-0.30018
N2	-0.41709	0.146676	1.502278
C3	3.588092	0.596157	-0.06233
O4	3.856546	-0.31958	-0.85778
C5	-1.53883	-0.26396	0.898493
O6	2.467491	1.016947	0.361246
N7	-1.42084	-0.07967	-0.41032
C8	0.590263	1.174325	-3.04824
O9	1.275815	0.422961	-2.30266
O10	-0.23354	2.038745	-2.65599
C11	0.716194	0.978919	-4.57542
F12	-0.42267	0.414829	-5.02768
F13	0.874965	2.159982	-5.18636
F14	1.739293	0.185541	-4.89476
C15	4.778883	1.382428	0.552101
F16	4.667763	2.69195	0.263695
F17	4.774466	1.246637	1.892253
F18	5.952459	0.945954	0.088942
H19	-0.06301	2.058066	-1.29545
C20	-4.90384	-1.98769	2.920156
C21	-4.36858	-2.61976	1.799019
C22	-3.27864	-2.05373	1.146599
C23	-2.70884	-0.85299	1.587078

C24	-3.26365	-0.24004	2.715706
C25	-4.35106	-0.79421	3.381956
F26	-5.94383	-2.52511	3.551564
F27	-4.89372	-3.76601	1.36477
F28	-2.77296	-2.6948	0.089072
F29	-2.75694	0.909966	3.173605
F30	-4.86771	-0.18904	4.452267
C31	1.192099	-1.05076	5.203457
C32	0.599186	-2.00236	4.377417
C33	0.056962	-1.61531	3.157114
C34	0.064804	-0.27432	2.739133
C35	0.676789	0.659545	3.589499
C36	1.235965	0.28399	4.805263
F37	1.716798	-1.4158	6.372806
F38	0.564208	-3.28378	4.752274
F39	-0.47641	-2.56003	2.370723
F40	0.725093	1.947112	3.232327
F41	1.801921	1.194643	5.59932
C42	-4.34114	-0.14953	-3.4369
C43	-4.60053	0.517036	-2.24167
C44	-3.63889	0.533882	-1.23842
C45	-2.41482	-0.1366	-1.38015
C46	-2.18195	-0.79707	-2.59379
C47	-3.12179	-0.79931	-3.61707
F48	-5.25572	-0.16234	-4.40668
F49	-5.76174	1.153673	-2.06895
F50	-3.89068	1.225872	-0.11564
F51	-1.01107	-1.418	-2.79458
F52	-2.86529	-1.42801	-4.76425
O53	0.850951	-1.70062	-0.21411
C54	1.447357	-2.44935	-1.00572
O55	2.522799	-2.22444	-1.65317
C56	0.849381	-3.86279	-1.20615
F57	1.194794	-4.37368	-2.39002
F58	1.305693	-4.67334	-0.23479
F59	-0.48671	-3.81583	-1.1281
H60	3.007704	-1.31895	-1.35601
C61	0.160422	2.637833	-0.1128
H62	0.999757	3.262997	-0.42092
H63	-0.80279	3.129035	-0.29691

H64	0.214888	2.472275	0.95977

Table S50. [$Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}$-H-$TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.529239	0.325283	-0.3185
N2	-0.45217	0.03018	1.485797
C3	3.578141	0.793381	-0.12382
O4	3.983337	-0.08696	-0.94155
C5	-1.58778	-0.35078	0.890536
O6	2.433558	0.990111	0.331022
N7	-1.45971	-0.1806	-0.42077
C8	0.570008	1.07375	-3.07781
O9	1.230527	0.317687	-2.32048
O10	-0.2463	1.956245	-2.69773
C11	0.713409	0.882082	-4.60333
F12	-0.45187	0.408761	-5.08662
F13	0.973415	2.055683	-5.19585
F14	1.683674	0.020153	-4.90616
C15	4.691018	1.72335	0.421967
F16	5.656228	1.905285	-0.48373
F17	4.19018	2.916503	0.762895
F18	5.229224	1.156812	1.517914
H19	-0.11159	1.978276	-1.38383
C20	-5.02942	-1.89199	2.929804
C21	-4.56486	-2.52379	1.777613
C22	-3.44964	-2.01786	1.118696
C23	-2.78198	-0.87787	1.584151
C24	-3.26966	-0.26254	2.743601
C25	-4.38112	-0.75795	3.416035
F26	-6.09337	-2.37206	3.56693
F27	-5.18207	-3.61293	1.318913
F28	-3.01719	-2.65844	0.029379
F29	-2.67521	0.833562	3.227108
F30	-4.83096	-0.15133	4.515257
C31	1.264677	-1.3266	5.079402
C32	0.572326	-2.22671	4.273321
C33	-0.0087	-1.7892	3.088089
C34	0.058725	-0.44314	2.690544
C35	0.770262	0.43794	3.519258
C36	1.369083	0.009692	4.697786

F37	1.82712	-1.74244	6.213967
F38	0.480132	-3.50931	4.632931
F39	-0.63914	-2.6869	2.321439
F40	0.882851	1.724607	3.170993
F41	2.032811	0.871398	5.471345
C42	-4.40185	0.130472	-3.4078
C43	-4.59004	0.770313	-2.18493
C44	-3.61885	0.665732	-1.19683
C45	-2.46135	-0.10565	-1.3811
C46	-2.29507	-0.73189	-2.62375
C47	-3.24431	-0.6125	-3.63178
F48	-5.32497	0.234355	-4.36353
F49	-5.6895	1.497831	-1.97169
F50	-3.79334	1.339054	-0.04757
F51	-1.18201	-1.43422	-2.86133
F52	-3.05669	-1.21281	-4.80704
O53	0.843948	-1.75542	-0.18855
C54	1.685438	-2.45494	-0.8173
O55	2.748879	-2.11421	-1.3765
C56	1.29676	-3.9558	-0.88301
F57	2.267038	-4.70049	-1.41822
F58	1.03474	-4.42016	0.352572
F59	0.186685	-4.10021	-1.63029
H60	3.298204	-0.94008	-1.17359
C61	-0.00846	2.520067	-0.13493
H62	0.653307	3.293422	-0.53689
H63	-1.05701	2.831939	-0.17342
H64	0.250727	2.394168	0.913739

Table S51. $[Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.286048	0.484272	-0.09171
N2	-0.58037	-0.2548	1.677662
C3	3.306602	0.982035	0.070264
O4	3.688609	0.181709	-0.81145
C5	-1.73132	-0.52933	1.072265
O6	2.159801	1.147573	0.569112
N7	-1.67553	-0.14262	-0.1995
C8	4.395639	1.896765	0.691271
F9	3.896985	3.104142	0.992734

F10	4.850426	1.33034	1.826383
F11	5.426722	2.058853	-0.14336
H12	0.774174	2.064435	-1.47948
C13	-5.13397	-2.33543	2.952379
C14	-4.63292	-2.87208	1.767324
C15	-3.52904	-2.28249	1.161324
C16	-2.90801	-1.1583	1.716423
C17	-3.42551	-0.64219	2.909689
C18	-4.53133	-1.21779	3.526612
F19	-6.19001	-2.89372	3.538021
F20	-5.20617	-3.94921	1.228264
F21	-3.05584	-2.82529	0.034532
F22	-2.86606	0.429248	3.477825
F23	-5.01739	-0.70407	4.657261
C24	1.212675	-2.06107	5.019984
C25	0.533521	-2.85301	4.097294
C26	-0.07374	-2.26014	2.996765
C27	-0.04935	-0.86904	2.801601
C28	0.654224	-0.09719	3.739871
C29	1.279973	-0.68145	4.835642
F30	1.800854	-2.62349	6.07658
F31	0.481678	-4.17798	4.263396
F32	-0.68239	-3.0501	2.099186
F33	0.732475	1.223163	3.578961
F34	1.936672	0.073283	5.71939
C35	-4.78242	0.233177	-3.00626
C36	-4.87999	0.883809	-1.77837
C37	-3.85353	0.756274	-0.84852
C38	-2.72345	-0.03366	-1.10658
C39	-2.65325	-0.67956	-2.34984
C40	-3.66362	-0.54618	-3.29512
F41	-5.75977	0.353282	-3.90466
F42	-5.9488	1.635809	-1.5046
F43	-3.95255	1.402322	0.320318
F44	-1.59532	-1.44706	-2.6403
F45	-3.57699	-1.17345	-4.47004
O46	-0.35763	2.326944	0.550827
C47	0.110565	3.322079	-0.06429
O48	0.801983	3.279379	-1.11412
C49	-0.25546	4.717125	0.48936

F50	-1.31893	5.182446	-0.19265
F51	-0.56975	4.660667	1.78485
F52	0.762771	5.566568	0.324442
O53	0.660164	-1.55848	-0.46792
C54	1.521306	-2.2478	-1.04174
O55	2.665901	-1.91071	-1.47979
C56	1.128987	-3.73292	-1.24805
F57	2.11707	-4.43616	-1.80249
F58	0.820564	-4.27866	-0.06084
F59	0.049845	-3.80008	-2.04338
H60	3.018433	-0.9104	-1.1909
C61	0.773177	0.944312	-2.30275
H62	0.311775	-0.02223	-2.50023
H63	0.270341	1.632114	-2.99511
H64	1.835143	0.893098	-2.55006

Table S52. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.254128	0.3812	-0.1115
N2	-0.59167	-0.35593	1.668164
C3	3.313937	1.141151	0.048132
O4	3.84594	0.353181	-0.80546
C5	-1.75409	-0.60199	1.074095
O6	2.168432	1.116961	0.522412
N7	-1.69011	-0.22867	-0.20198
C8	4.272986	2.24902	0.549044
F9	3.602254	3.191903	1.214117
F10	5.189037	1.708476	1.369188
F11	4.904455	2.814535	-0.48758
H12	0.692754	1.959043	-1.51891
C13	-5.22967	-2.20311	3.003172
C14	-4.78032	-2.7694	1.810943
C15	-3.65101	-2.24972	1.187789
C16	-2.9529	-1.16694	1.73325
C17	-3.42028	-0.61937	2.933781
C18	-4.55016	-1.12517	3.567731
F19	-6.30992	-2.69439	3.604389
F20	-5.42819	-3.80791	1.281018
F21	-3.23119	-2.81948	0.054085
F22	-2.79001	0.416734	3.492855

F23	-4.98647	-0.58157	4.704728
C24	1.200081	-2.26052	4.956811
C25	0.457917	-3.01444	4.050946
C26	-0.14828	-2.38951	2.967459
C27	-0.06035	-1.0002	2.774767
C28	0.705822	-0.26804	3.695479
C29	1.330964	-0.88531	4.773034
F30	1.787572	-2.85484	5.996341
F31	0.344028	-4.33509	4.217351
F32	-0.82163	-3.14536	2.089049
F33	0.848503	1.048254	3.532866
F34	2.048304	-0.16576	5.639638
C35	-4.77788	0.315323	-2.99824
C36	-4.83013	0.981263	-1.77551
C37	-3.80863	0.798751	-0.84979
C38	-2.73147	-0.06188	-1.10741
C39	-2.70504	-0.72285	-2.34474
C40	-3.71075	-0.5343	-3.28623
F41	-5.75016	0.488288	-3.89313
F42	-5.84983	1.799291	-1.50382
F43	-3.86081	1.458013	0.313975
F44	-1.69767	-1.5532	-2.63201
F45	-3.6698	-1.17374	-4.45673
O46	-0.39315	2.244037	0.54195
C47	0.072606	3.230805	-0.08319
O48	0.734961	3.177232	-1.15437
C49	-0.16358	4.63289	0.520492
F50	-0.6295	5.465125	-0.42216
F51	-1.03724	4.593291	1.528779
F52	1.004106	5.111526	0.976993
O53	0.63348	-1.61706	-0.48405
C54	1.639124	-2.21014	-0.97096
O55	2.743338	-1.76206	-1.32908
C56	1.390166	-3.73656	-1.11866
F57	2.466611	-4.3706	-1.58899
F58	1.074323	-4.26319	0.079875
F59	0.363278	-3.95555	-1.9584
H60	3.263548	-0.52106	-1.04181
C61	0.70627	0.827639	-2.33168
H62	0.242899	-0.14051	-2.51553

H63	0.205377	1.512972	-3.02809
H64	1.76527	0.766386	-2.59037

Table S53. [$Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})(CH_3{}^{eq}$-H-$TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.386403	0.348124	-0.19822
N2	-0.58124	-0.2322	1.557226
C3	3.110464	1.235093	-0.08627
O4	2.902434	1.68876	-1.24048
C5	-1.74094	-0.45164	0.94604
O6	2.284382	0.592375	0.61331
N7	-1.67027	-0.07534	-0.32837
C15	4.498986	1.514491	0.5283
F16	4.584652	1.056483	1.780612
F17	5.449133	0.930113	-0.21236
F18	4.718815	2.840703	0.541307
H19	-0.90979	2.314101	-1.79327
C20	-5.2245	-2.0551	2.860788
C21	-4.70027	-2.69106	1.735999
C22	-3.57346	-2.16394	1.113771
C23	-2.95006	-1.00984	1.59894
C24	-3.49294	-0.39118	2.729174
C25	-4.62358	-0.90013	3.359305
F19	-6.30361	-2.55176	3.45998
F20	-5.27516	-3.79993	1.268685
F21	-3.08248	-2.79254	0.042882
F22	-2.93351	0.719588	3.2193
F23	-5.13572	-0.28878	4.428473
C31	1.133401	-2.14491	4.878101
C32	0.436277	-2.90287	3.939887
C33	-0.15232	-2.27613	2.847832
C34	-0.08565	-0.88372	2.680117
C35	0.632194	-0.14617	3.633403
C36	1.236215	-0.76371	4.72203
F30	1.700506	-2.74095	5.927487
F31	0.344794	-4.22702	4.087633
F32	-0.79271	-3.02856	1.945425
F33	0.742333	1.176152	3.495243
F34	1.90437	-0.0412	5.624782
C42	-4.89417	0.290747	-3.00956

C43	-4.86045	1.068046	-1.8531
C44	-3.79084	0.939979	-0.97478
C45	-2.74792	0.030586	-1.20697
C46	-2.80317	-0.73233	-2.38272
C47	-3.86083	-0.60533	-3.27863
F41	-5.91255	0.407354	-3.86123
F42	-5.84183	1.937506	-1.60227
F43	-3.75114	1.711111	0.124031
F44	-1.8252	-1.59937	-2.65591
F45	-3.8982	-1.34691	-4.38679
O53	-0.04231	2.392681	0.407009
C54	-0.78666	3.195042	-0.13911
O55	-1.26762	3.114104	-1.35739
C56	-1.28832	4.451767	0.60869
F57	-0.6593	4.576717	1.772208
F58	-1.07318	5.543427	-0.13437
F59	-2.60543	4.324751	0.824663
O60	0.638909	-1.61726	-0.47585
C61	1.735046	-2.09364	-0.99378
O62	2.691488	-1.50679	-1.4614
C63	1.682389	-3.64879	-0.95598
F64	2.822139	-4.17784	-1.41008
F65	1.486958	-4.08842	0.304534
F66	0.670571	-4.10935	-1.7175
H67	1.787699	1.171612	-1.62155
C62	0.785837	0.747418	-2.46472
H62	0.01658	-0.01017	-2.61203
H63	0.465748	1.698593	-2.91145
H64	1.634449	0.38331	-3.05535

Table S54. [$Rh^{III\text{-}I}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Atom	x	y	z
Rh1	0.553237	0.127281	-0.35355
N2	-0.32453	-0.23989	1.476501
C3	3.149705	1.544968	-0.01078
O4	2.653954	2.673822	-0.24364
C5	-1.54984	-0.43094	0.987001
O6	2.586932	0.42668	0.109438
N7	-1.52647	-0.25184	-0.33618
C8	0.884957	1.456441	-3.09619

O9	1.110124	0.470056	-2.40381
O10	0.256602	2.551868	-2.78816
C11	1.370915	1.475732	-4.56274
F12	0.31821	1.589253	-5.39434
F13	2.183549	2.526124	-4.77152
F14	2.032089	0.358259	-4.86468
C15	4.693035	1.472056	0.138599
F16	5.269684	2.680026	0.035288
F17	5.029734	0.956264	1.337148
F18	5.22413	0.68015	-0.81475
H19	1.451981	3.146992	0.375702
C20	-4.97734	-1.46986	3.364639
C21	-4.65825	-2.22488	2.239606
C22	-3.54574	-1.88551	1.476106
C23	-2.73504	-0.79555	1.806596
C24	-3.07934	-0.05511	2.942083
C25	-4.18502	-0.38181	3.719442
F26	-6.0437	-1.78923	4.103791
F27	-5.41623	-3.27558	1.905961
F28	-3.26113	-2.6409	0.410011
F29	-2.35124	1.007902	3.303968
F30	-4.49846	0.349656	4.795487
C31	1.263288	-1.3927	5.197757
C32	0.455651	-2.28167	4.495669
C33	-0.08158	-1.90476	3.269923
C34	0.144903	-0.63052	2.724297
C35	0.975509	0.237696	3.449134
C36	1.529468	-0.133	4.668349
F37	1.77911	-1.74481	6.383044
F38	0.20521	-3.49449	5.001082
F39	-0.82216	-2.79508	2.597043
F40	1.239061	1.457447	2.968085
F41	2.303	0.723625	5.349549
C42	-4.66483	0.226511	-3.11906
C43	-4.7965	0.761168	-1.84323
C44	-3.77589	0.609423	-0.91092
C45	-2.59749	-0.10711	-1.19643
C46	-2.4932	-0.61753	-2.50509
C47	-3.49962	-0.45843	-3.4499
F48	-5.64651	0.371882	-4.02011

F49	-5.90441	1.443035	-1.51722
F50	-3.94448	1.195994	0.285748
F51	-1.38613	-1.27899	-2.87126
F52	-3.36082	-0.97617	-4.67744
O53	-0.90872	3.041636	-0.51884
C54	-0.50678	3.414376	0.582356
O55	0.703941	3.552709	0.999535
C56	-1.53945	3.833871	1.658345
F57	-1.7075	5.173691	1.618191
F58	-2.72774	3.260279	1.435438
F59	-1.13071	3.502606	2.890282
C60	1.096725	-2.16089	-0.62757
H61	2.133918	-1.88734	-0.74449
H62	0.734824	-2.45165	0.34552
H63	0.459177	-2.23993	-1.49368
H64	-0.08304	2.61197	-1.83384
O65	1.623196	-4.08184	-0.97004
C66	1.648925	-4.77799	0.100269
O67	1.43081	-4.46394	1.270869
C68	2.065407	-6.25927	-0.17021
F69	1.671052	-6.70829	-1.38098
F70	3.414853	-6.38944	-0.11823
F71	1.551933	-7.10042	0.750792

Table S55. $[Rh^{III\text{-}I}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFAH)]^{‡}$

Atom	x	y	z
Rh1	0.360921	0.233328	-0.20482
N2	-0.49879	-0.05082	1.661678
C3	3.278649	-0.06911	0.787986
O4	3.415466	-1.30618	0.663933
C5	-1.72756	-0.21813	1.168387
O6	2.394354	0.69888	0.316678
N7	-1.68742	-0.06318	-0.15589
C8	0.511799	1.166657	-3.1181
O9	0.780097	0.27553	-2.31613
O10	0.262184	2.418341	-2.87297
C11	0.358365	0.809739	-4.61213
F12	0.792707	1.797673	-5.39901
F13	1.039353	-0.30427	-4.8951
F14	-0.94585	0.59588	-4.87348

C15	4.308873	0.613175	1.729414
F16	5.491654	-0.00687	1.696488
F17	4.493325	1.901939	1.399485
F18	3.838803	0.567579	2.994626
H19	2.143241	2.374416	0.706261
C20	-5.1808	-1.29527	3.481183
C21	-4.84829	-2.02439	2.341546
C22	-3.72882	-1.66283	1.600668
C23	-2.92599	-0.57539	1.963462
C24	-3.28235	0.138342	3.112236
C25	-4.39782	-0.2091	3.867283
F26	-6.24774	-1.6397	4.200083
F27	-5.59264	-3.07119	1.977863
F28	-3.41777	-2.39821	0.524563
F29	-2.5542	1.190478	3.504909
F30	-4.72593	0.49562	4.953585
C31	0.990273	-1.31822	5.395357
C32	0.224283	-2.19138	4.626759
C33	-0.27404	-1.76985	3.400025
C34	-0.05969	-0.47026	2.913239
C35	0.731104	0.377468	3.70277
C36	1.248456	-0.03382	4.926151
F37	1.479808	-1.71409	6.572915
F38	-0.00861	-3.43657	5.05756
F39	-0.94995	-2.65739	2.645543
F40	1.00105	1.61429	3.275915
F41	1.984426	0.804132	5.660261
C42	-4.79616	0.676628	-2.9004
C43	-4.83098	1.279739	-1.64593
C44	-3.81604	1.031798	-0.72774
C45	-2.75439	0.155417	-1.01018
C46	-2.74892	-0.42818	-2.28592
C47	-3.73979	-0.17271	-3.22331
F48	-5.76624	0.911756	-3.78787
F49	-5.82736	2.11393	-1.33305
F50	-3.84839	1.685406	0.445602
F51	-1.74797	-1.25804	-2.62592
F52	-3.69497	-0.75342	-4.42593
O53	0.409642	3.6106	-0.54162
C54	0.974668	3.90158	0.498694

O55	1.942965	3.26564	1.103746
C56	0.536625	5.147777	1.303251
F57	1.587925	5.779039	1.840833
F58	-0.12017	6.001857	0.513766
F59	-0.28455	4.759266	2.295509
C60	0.676582	-2.41117	-0.57341
H61	1.225271	-1.88098	-1.33866
H62	0.977067	-2.28019	0.455091
H63	-0.37891	-2.54777	-0.76142
H64	0.350852	2.672003	-1.9065
O65	1.204413	-3.9962	-0.86872
C66	2.448631	-4.18342	-0.86533
O67	3.378047	-3.3769	-0.56156
C68	2.921217	-5.60577	-1.26144
F69	2.050365	-6.17185	-2.09846
F70	4.121906	-5.55942	-1.84062
F71	3.001384	-6.34657	-0.14539
H72	3.226058	-2.39646	-0.09412

Table S56. $[Rh^{III\text{-}II}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Atom	x	y	z
Rh1	0.468745	-0.09168	-0.09026
N2	-0.39146	-0.36057	1.739238
C3	3.010919	1.314071	0.58318
O4	2.708711	2.327371	-0.11168
C5	-1.61837	-0.57358	1.260543
O6	2.480106	0.179636	0.54145
N7	-1.55448	-0.55743	-0.0729
C8	1.209606	1.009469	-2.88124
O9	0.816752	0.060573	-2.19691
O10	1.862073	2.058234	-2.51163
C11	0.848987	0.972446	-4.385
F12	1.40659	1.977219	-5.06069
F13	1.244256	-0.18842	-4.91709
F14	-0.48955	1.064866	-4.49799
C15	4.176701	1.478571	1.591904
F16	4.239457	2.738871	2.039516
F17	4.023079	0.661048	2.645676
F18	5.339091	1.178278	0.988688
H19	1.538132	3.340598	0.523971

C20	-5.13401	-1.27671	3.615026
C21	-4.84898	-2.09663	2.524783
C22	-3.70735	-1.85818	1.767633
C23	-2.83077	-0.81042	2.073864
C24	-3.14088	-0.00356	3.174894
C25	-4.27751	-0.22735	3.943335
F26	-6.22364	-1.4974	4.344659
F27	-5.66282	-3.10754	2.219052
F28	-3.45197	-2.67165	0.737513
F29	-2.34514	1.017735	3.509068
F30	-4.55428	0.559753	4.983545
C31	1.309628	-1.00871	5.523116
C32	0.484737	-1.98477	4.967374
C33	-0.08912	-1.7709	3.719546
C34	0.112817	-0.57719	3.013015
C35	0.954401	0.380987	3.592693
C36	1.553643	0.175316	4.828303
F37	1.867505	-1.2084	6.717018
F38	0.264189	-3.1261	5.623423
F39	-0.83155	-2.74603	3.166994
F40	1.188361	1.530568	2.937916
F41	2.344307	1.107844	5.359521
C42	-4.46771	0.30697	-2.9776
C43	-4.50233	0.978886	-1.75844
C44	-3.55544	0.689943	-0.78269
C45	-2.57181	-0.29226	-0.97947
C46	-2.55703	-0.94605	-2.22133
C47	-3.48623	-0.65428	-3.21222
F48	-5.37115	0.583541	-3.91862
F49	-5.43325	1.910749	-1.53613
F50	-3.58977	1.38432	0.364675
F51	-1.62259	-1.87211	-2.46528
F52	-3.4531	-1.29824	-4.3804
O53	-0.45504	2.199792	-0.16257
C54	-0.35793	3.242049	0.468608
O55	0.737401	3.851531	0.836367
C56	-1.6442	3.964166	0.935185
F57	-1.40652	5.209361	1.352161
F58	-2.52638	4.004411	-0.07211
F59	-2.18471	3.265926	1.950145

C60	0.928985	-2.44469	-0.17574
H61	1.951812	-2.15895	0.03252
H62	0.287235	-2.72223	0.647569
H63	0.516787	-2.37832	-1.17369
H64	2.123926	2.082077	-1.51616
O65	1.406972	-4.2949	-0.48188
V66	2.673637	-4.70546	-1.43753
Cl67	2.720880	-6.83007	-1.8117
Cl68	2.402778	-3.60692	-3.29383
Cl69	4.467684	-4.02386	-0.41528

Table S57. $[Rh^{IV\text{-}II}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Atom	x	y	z
Rh1	0.662122	0.396177	-0.3603
N2	-0.08205	-0.89335	1.09911
C3	3.373181	1.490495	0.361704
O4	3.047159	2.681509	0.478224
C5	-1.343	-0.79497	0.668942
O6	2.685262	0.453274	0.114967
N7	-1.3828	-0.08705	-0.45069
C8	0.381018	2.089862	-2.7942
O9	1.068324	1.890074	-1.72101
O10	-0.42472	1.361971	-3.35871
C11	0.705053	3.477726	-3.42269
F12	1.820115	3.401299	-4.18479
F13	-0.29788	3.896992	-4.21427
F14	0.913943	4.428539	-2.49274
C15	4.874622	1.145145	0.567078
F16	5.61288	2.236222	0.818819
F17	5.025278	0.298194	1.608347
F18	5.382711	0.545278	-0.5267
H19	1.726387	3.372726	0.391096
C20	-4.76293	-2.4195	2.692111
C21	-3.67965	-3.24175	2.394626
C22	-2.57373	-2.7134	1.733764
C23	-2.52835	-1.36718	1.357588
C24	-3.62874	-0.56156	1.670928
C25	-4.74012	-1.0752	2.329819
F26	-5.82484	-2.9193	3.330066
F27	-3.70875	-4.53235	2.743851

F28	-1.55184	-3.52386	1.466171
F29	-3.62917	0.737112	1.35754
F30	-5.77784	-0.28488	2.628848
C31	1.38436	-1.80669	4.93331
C32	0.281651	-0.96848	4.807237
C33	-0.21816	-0.67095	3.544664
C34	0.345107	-1.21435	2.378135
C35	1.468559	-2.04454	2.535425
C36	1.982617	-2.33882	3.794087
F37	1.869903	-2.0986	6.146727
F38	-0.28439	-0.4381	5.901076
F39	-1.25475	0.177485	3.459876
F40	2.060264	-2.56505	1.464052
F41	3.043717	-3.14402	3.922327
C42	-4.58865	0.258891	-3.14861
C43	-3.94194	1.396089	-2.67228
C44	-2.89646	1.270399	-1.7667
C45	-2.46122	0.015777	-1.31854
C46	-3.11981	-1.11328	-1.8286
C47	-4.17663	-1.00016	-2.72454
F48	-5.61069	0.377151	-4.00607
F49	-4.34794	2.605538	-3.0759
F50	-2.30789	2.380625	-1.31199
F51	-2.72823	-2.33942	-1.45206
F52	-4.7956	-2.09707	-3.18316
O53	-0.21435	2.087378	1.064875
C54	-0.13769	3.297321	0.876857
O55	0.890742	3.981112	0.500012
C56	-1.38436	4.182663	1.114963
F57	-1.66382	4.915631	0.025486
F58	-2.45333	3.434346	1.408875
F59	-1.16786	5.0289	2.143225
C60	1.112825	-1.08547	-1.86018
H61	2.158873	-0.89691	-2.06959
H62	0.858127	-1.8533	-1.1161
H63	0.41468	-0.88804	-2.66274
O64	1.448165	-3.11209	-2.79911
C65	0.927516	-3.98371	-2.03175
O66	0.37752	-3.87738	-0.93633
C67	1.083655	-5.43476	-2.61046

F68	2.291519	-5.93591	-2.26861
F69	0.14688	-6.26323	-2.11793
F70	0.993428	-5.47314	-3.95328

Table S58. $[Rh^{IV\text{-}II}(NN^{F})(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Atom	x	y	z
Rh1	0.322385	0.031697	-0.25187
N2	-0.45903	-0.4006	1.590699
C3	3.40724	0.263199	0.114527
O4	3.762206	-0.39389	-0.86872
C5	-1.69085	-0.61226	1.121727
O6	2.246518	0.747891	0.357318
N7	-1.65749	-0.51444	-0.20834
C8	1.325847	-0.03646	-3.23273
O9	0.52743	0.329024	-2.35903
O10	2.557984	-0.37934	-3.11165
C11	0.813563	-0.01015	-4.69187
F12	1.571036	-0.74334	-5.50125
F13	-0.44809	-0.45018	-4.74278
F14	0.834716	1.269869	-5.11856
C15	4.418883	0.526317	1.259133
F16	5.647809	0.122307	0.948573
F17	4.453167	1.839374	1.555931
F18	4.012686	-0.13878	2.362533
H19	1.856125	2.268082	0.890532
C20	-5.15212	-1.43352	3.512221
C21	-4.90048	-2.19234	2.370351
C22	-3.77599	-1.91973	1.598661
C23	-2.88454	-0.89689	1.944342
C24	-3.16157	-0.14965	3.09599
C25	-4.28149	-0.40805	3.877687
F26	-6.22565	-1.68735	4.254271
F27	-5.73073	-3.17739	2.028093
F28	-3.55401	-2.66995	0.515546
F29	-2.3535	0.850959	3.461782
F30	-4.53	0.323322	4.964457
C31	1.247435	-1.70484	5.207198
C32	0.43843	-2.57118	4.474787
C33	-0.1287	-2.13618	3.283402
C34	0.06774	-0.83179	2.802973

C35	0.89484	0.01305	3.55583
C36	1.481501	-0.41189	4.742456
F37	1.796894	-2.11279	6.350322
F38	0.2244	-3.81457	4.909481
F39	-0.86755	-2.99952	2.565884
F40	1.119364	1.262901	3.135585
F41	2.252361	0.41649	5.447825
C42	-4.63112	0.605427	-2.95353
C43	-4.59066	1.222267	-1.70489
C44	-3.62158	0.846754	-0.78287
C45	-2.69372	-0.16717	-1.06816
C46	-2.75214	-0.76585	-2.33558
C47	-3.70487	-0.38607	-3.27316
F48	-5.5568	0.964246	-3.84251
F49	-5.47112	2.180564	-1.40413
F50	-3.57363	1.485469	0.395253
F51	-1.87523	-1.71973	-2.65174
F52	-3.74757	-0.9734	-4.46918
O53	-0.39903	2.230996	0.052195
C54	0.199136	3.154727	0.591541
O55	1.427481	3.163288	1.0255
C56	-0.50917	4.509127	0.834292
F57	0.179664	5.500714	0.251836
F58	-1.74501	4.487446	0.333609
F59	-0.57835	4.750113	2.152567
C60	0.872922	-2.09185	-0.47692
H61	1.952289	-2.03617	-0.40748
H62	0.362875	-2.62296	0.316236
H63	0.40448	-2.07409	-1.46198
H64	2.936747	-0.37988	-2.15564
O65	1.294995	-4.04905	-1.35784
C66	1.238956	-3.94433	-2.63703
O67	0.952456	-2.99366	-3.35104
C68	1.604255	-5.32546	-3.30515
F69	2.817277	-5.73943	-2.90502
F70	0.701756	-6.2596	-2.96061
F71	1.6118	-5.21509	-4.63503

Table S59. [$Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_2TFA^{ax}$-H-$TFA^{eq})]^{‡}$

Atom	x	y	z

Rh1	0.420306	0.607544	-0.3537
N2	-0.56583	0.28621	1.455073
C3	3.402375	0.952094	-0.07692
O4	3.728007	0.096574	-0.91744
C5	-1.65383	-0.21789	0.858165
O6	2.25274	1.284227	0.346851
N7	-1.55812	-0.03089	-0.45241
C8	0.319535	1.330704	-3.09535
O9	1.089435	0.651389	-2.35914
O10	-0.59172	2.094467	-2.69068
C11	0.453288	1.15536	-4.62474
F12	-0.61083	0.450656	-5.06372
F13	0.452122	2.34612	-5.23491
F14	1.56424	0.497477	-4.95721
C15	4.570949	1.696017	0.626111
F16	4.166747	2.833284	1.21293
F17	5.074221	0.890576	1.583089
F18	5.545492	1.985531	-0.23992
H19	-0.38323	2.14235	-1.3105
C20	-4.8307	-2.22538	2.920025
C21	-4.25249	-2.81204	1.795235
C22	-3.22679	-2.1518	1.127691
C23	-2.76433	-0.90166	1.556565
C24	-3.35996	-0.33561	2.688969
C25	-4.38459	-0.98333	3.370161
F26	-5.809	-2.85258	3.566031
F27	-4.6741	-4.00406	1.37264
F28	-2.6751	-2.7501	0.068405
F29	-2.95359	0.857368	3.13589
F30	-4.9417	-0.42295	4.44397
C31	1.10659	-0.77027	5.170291
C32	0.61034	-1.77056	4.337282
C33	0.050514	-1.43133	3.111182
C34	-0.05444	-0.09414	2.694917
C35	0.462077	0.891003	3.550767
C36	1.037151	0.564386	4.773736
F37	1.646386	-1.08921	6.345608
F38	0.682596	-3.05017	4.712166
F39	-0.39175	-2.41786	2.319764
F40	0.397903	2.17497	3.191794

F41	1.509669	1.518639	5.576044
C42	-4.49429	-0.42949	-3.43812
C43	-4.79608	0.242318	-2.25548
C44	-3.82577	0.369967	-1.26884
C45	-2.54995	-0.19447	-1.41352
C46	-2.27483	-0.86214	-2.61363
C47	-3.22435	-0.97348	-3.62173
F48	-5.41723	-0.54916	-4.39175
F49	-6.00742	0.774963	-2.07866
F50	-4.12198	1.061794	-0.1569
F51	-1.05716	-1.38407	-2.81581
F52	-2.92904	-1.60786	-4.75586
O53	0.813998	-1.47737	-0.25268
C54	1.472358	-2.1864	-1.03688
O55	2.518983	-1.88348	-1.69363
C56	0.99519	-3.65012	-1.20416
F57	1.364651	-4.14534	-2.38685
F58	1.538288	-4.40043	-0.22993
F59	-0.33782	-3.7193	-1.10258
H60	2.948503	-0.93737	-1.40895
C61	-0.09735	2.825554	-0.20725
H63	-1.06373	3.318863	-0.38122
H64	0.008835	2.711308	0.869725
O64	0.955602	3.62692	-0.74712
C65	1.694947	4.336987	0.124748
O66	1.48176	4.491521	1.295717
C67	2.881999	4.9731	-0.63276
F68	3.576802	4.031727	-1.30195
F69	2.430277	5.871163	-1.52601
F70	3.699962	5.587152	0.218527

Table S60. [$Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_2TFA^{ax}$-H-$TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.548951	0.364872	-0.43124
N2	-0.46022	0.212252	1.360289
C3	3.624581	0.726972	-0.23605
O4	3.999567	-0.22175	-0.99137
C5	-1.60642	-0.1752	0.777221
O6	2.48489	1.00031	0.190421
N7	-1.45008	-0.10018	-0.53911

C8	0.751103	1.064489	-3.20378
O9	1.313598	0.261648	-2.41372
O10	-0.00444	2.012992	-2.86397
C11	0.949405	0.844237	-4.72011
F12	-0.20949	0.397831	-5.24209
F13	1.269086	1.998728	-5.31942
F14	1.90424	-0.05194	-4.96957
C15	4.787667	1.639807	0.229577
F16	4.32686	2.742733	0.825164
F17	5.553706	0.965479	1.102624
F18	5.541699	1.997005	-0.81778
H19	0.079641	2.050337	-1.53137
C20	-5.10677	-1.34713	2.95416
C21	-4.72782	-2.06337	1.819957
C22	-3.59138	-1.68328	1.115488
C23	-2.81625	-0.58765	1.514856
C24	-3.21546	0.108093	2.663961
C25	-4.34786	-0.25927	3.380339
F26	-6.19053	-1.70707	3.634161
F27	-5.44777	-3.113	1.424073
F28	-3.24223	-2.40478	0.045909
F29	-2.50908	1.153404	3.103603
F30	-4.70888	0.424284	4.465797
C31	1.235498	-1.07829	4.98761
C32	0.492618	-1.97703	4.226142
C33	-0.0801	-1.56141	3.029401
C34	0.044931	-0.23712	2.577163
C35	0.804602	0.643887	3.362435
C36	1.397729	0.235294	4.550753
F37	1.79192	-1.47438	6.131599
F38	0.345401	-3.23811	4.639002
F39	-0.76074	-2.45898	2.30688
F40	0.972205	1.907065	2.960362
F41	2.112747	1.093165	5.280545
C42	-4.17834	-0.02119	-3.74403
C43	-4.4933	0.636772	-2.55808
C44	-3.60322	0.606651	-1.49118
C45	-2.39368	-0.10204	-1.56169
C46	-2.10833	-0.76312	-2.76626
C47	-2.97693	-0.71847	-3.84971

F48	-5.02473	0.013636	-4.77231
F49	-5.64262	1.306466	-2.45006
F50	-3.92991	1.266531	-0.37292
F51	-0.95837	-1.43603	-2.89385
F52	-2.66969	-1.3493	-4.983
O53	0.769942	-1.68926	-0.19718
C54	1.579973	-2.46058	-0.79075
O55	2.653839	-2.19869	-1.36369
C56	1.10985	-3.93995	-0.78497
F57	2.083489	-4.76965	-1.16516
F58	0.698035	-4.2974	0.443341
F59	0.074352	-4.07835	-1.63286
H60	3.281036	-1.03225	-1.1992
C61	0.114707	2.618215	-0.29613
H62	0.614135	3.451791	-0.80987
H64	0.59156	2.548678	0.679118
O64	-1.28622	2.933473	-0.14443
C65	-1.59265	3.760708	0.866164
O66	-0.82818	4.246316	1.657194
C67	-3.11715	4.024801	0.911288
F68	-3.65814	4.057015	-0.31469
F69	-3.73086	3.054865	1.620412
F70	-3.35083	5.191864	1.514605

Table S61. $[Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.422987	0.521704	-0.09377
N2	-0.44486	-0.18239	1.671488
C3	3.47411	0.700695	0.285925
O4	3.82504	-0.13276	-0.57284
C5	-1.61529	-0.41604	1.077418
O6	2.312339	1.055329	0.640504
N7	-1.58052	0.007373	-0.17686
C8	4.593249	1.449916	1.06135
F9	4.440103	2.778413	0.931441
F10	4.520307	1.140867	2.369497
F11	5.807583	1.117602	0.616061
H12	0.051109	1.796332	-1.78099
C13	-5.02624	-2.18387	2.971008
C14	-4.48699	-2.77426	1.828594

C15	-3.37734	-2.1986	1.21977
C16	-2.79343	-1.03429	1.729978
C17	-3.34714	-0.46354	2.880256
C18	-4.4583	-1.02595	3.500441
F19	-6.0869	-2.7294	3.559467
F20	-5.02918	-3.88734	1.333821
F21	-2.86119	-2.7918	0.140374
F22	-2.81748	0.648435	3.396845
F23	-4.98252	-0.46366	4.589763
C24	1.356629	-2.20704	4.884488
C25	0.67642	-2.93675	3.91175
C26	0.067897	-2.27062	2.855484
C27	0.094031	-0.86887	2.753095
C28	0.794926	-0.15946	3.742308
C29	1.420668	-0.81757	4.796402
F30	1.945272	-2.83862	5.899434
F31	0.622659	-4.26874	3.990504
F32	-0.55308	-2.99777	1.914777
F33	0.865646	1.167489	3.676905
F34	2.073172	-0.12595	5.73217
C35	-4.72954	0.424156	-2.92797
C36	-4.61556	1.317233	-1.86336
C37	-3.58063	1.162925	-0.94945
C38	-2.65338	0.119737	-1.06393
C39	-2.79173	-0.76089	-2.1425
C40	-3.81479	-0.61688	-3.07161
F41	-5.71863	0.565677	-3.80871
F42	-5.49529	2.311721	-1.73022
F43	-3.46608	2.03179	0.065518
F44	-1.90844	-1.75283	-2.29997
F45	-3.92792	-1.46998	-4.08879
O46	-0.11323	2.402797	0.521208
C47	-0.64389	3.111774	-0.37671
O48	-0.70748	2.820544	-1.60019
C49	-1.23721	4.470415	0.05844
F50	-2.4182	4.666803	-0.54053
F51	-1.40572	4.529523	1.380212
F52	-0.39681	5.448932	-0.31641
O53	0.653237	-1.53962	-0.48262
C54	1.459848	-2.35812	-0.94611

O55	2.679651	-2.19084	-1.28136
C56	0.952668	-3.81732	-1.06104
F57	1.57053	-4.47201	-2.04534
F58	1.215175	-4.4407	0.104794
F59	-0.3646	-3.84799	-1.27241
H60	3.081263	-1.24308	-1.024
C61	1.149763	1.067924	-2.28471
H63	1.091069	1.900885	-2.99967
H64	2.174686	1.047599	-1.92686
O64	0.983599	-0.16436	-3.02087
C65	-0.0346	-0.22758	-3.87702
O66	-0.84489	0.640005	-4.09175
C67	-0.02698	-1.57864	-4.62921
F68	0.39564	-2.5885	-3.84522
F69	-1.25366	-1.86289	-5.06994
F70	0.801156	-1.49724	-5.68497

Table S62. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{ax})]^{\ddagger}$

Atom	x	y	z
Rh1	0.451365	0.327592	-0.15237
N2	-0.53695	-0.27048	1.576521
C3	3.498836	0.978139	0.22768
O4	4.018159	0.258458	-0.69337
C5	-1.66429	-0.53336	0.914703
O6	2.338785	0.950704	0.667103
N7	-1.50863	-0.21846	-0.36461
C8	4.479201	1.982862	0.881917
F9	3.810764	3.033424	1.366804
F10	5.11694	1.370732	1.894273
F11	5.383179	2.411543	-0.00183
H12	1.252194	1.784172	-1.51701
C13	-5.2993	-1.96702	2.667929
C14	-4.78134	-2.60098	1.538994
C15	-3.59562	-2.14061	0.977736
C16	-2.91042	-1.04866	1.521361
C17	-3.44513	-0.4343	2.659907
C18	-4.63125	-0.8814	3.232003
F19	-6.43354	-2.4015	3.209612
F20	-5.4178	-3.64668	1.010309
F21	-3.11031	-2.7751	-0.09325

F22	-2.82733	0.611467	3.214508
F23	-5.13185	-0.27458	4.308569
C24	1.067299	-2.156	4.970262
C25	0.359648	-2.91291	4.03878
C26	-0.18368	-2.29436	2.919314
C27	-0.06724	-0.90849	2.715437
C28	0.660161	-0.17247	3.664393
C29	1.224314	-0.78426	4.778066
F30	1.595724	-2.7443	6.043368
F31	0.219517	-4.22904	4.216246
F32	-0.8262	-3.05056	2.019718
F33	0.824924	1.139287	3.494032
F34	1.906522	-0.06339	5.670749
C35	-4.44533	0.088885	-3.3483
C36	-4.5724	0.833139	-2.17772
C37	-3.59564	0.735358	-1.19312
C38	-2.49328	-0.11607	-1.34238
C39	-2.38485	-0.84789	-2.53184
C40	-3.34653	-0.75006	-3.52838
F41	-5.37355	0.180994	-4.29962
F42	-5.62286	1.639871	-2.00779
F43	-3.72308	1.461733	-0.07555
F44	-1.32996	-1.64609	-2.72068
F45	-3.22674	-1.45294	-4.65573
O46	-0.1586	2.262338	0.300432
C47	0.49649	3.172576	-0.26908
O48	1.343404	3.002869	-1.18991
C49	0.221942	4.61464	0.21594
F50	0.979763	5.495733	-0.43865
F51	-1.06932	4.91697	0.012631
F52	0.484723	4.704934	1.526652
O53	0.810735	-1.69928	-0.36161
C54	1.805675	-2.29286	-0.87379
O55	2.872763	-1.82263	-1.3106
C56	1.589229	-3.82894	-0.96544
F57	2.69141	-4.45599	-1.38142
F58	1.246765	-4.31853	0.239808
F59	0.593051	-4.09451	-1.82807
H60	3.424568	-0.57934	-0.98788
C61	1.00088	0.729926	-2.39985

H62	0.984273	-0.35119	-2.50378
H64	1.885582	1.086676	-2.94285
O64	-0.19423	1.228515	-3.05103
C65	-0.05051	2.108929	-4.04898
O66	0.976705	2.514849	-4.52572
C67	-1.45004	2.543454	-4.54174
F68	-2.21834	2.943666	-3.50877
F69	-1.34754	3.54363	-5.41248
F70	-2.07141	1.508768	-5.14481

Table S63. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.557627	0.533237	0.074393
N2	-0.58541	-0.11733	1.71107
C3	3.33441	1.070455	0.381544
O4	3.225822	1.68348	-0.70452
C5	-1.69173	-0.26734	1.008603
O6	2.412001	0.43593	0.970206
N7	-1.58205	0.387065	-0.16939
C15	4.700894	1.129149	1.100871
F16	5.693448	0.906496	0.234423
F17	4.858191	2.354674	1.63165
F18	4.776336	0.227653	2.08574
H19	-1.71653	2.11648	0.462738
C20	-5.22493	-2.31845	2.294801
C21	-4.50734	-2.80283	1.20162
C22	-3.35649	-2.13967	0.789897
C23	-2.90654	-0.9941	1.452925
C24	-3.63994	-0.52902	2.547359
C25	-4.79416	-1.17833	2.971953
F19	-6.32597	-2.94759	2.694219
F20	-4.9211	-3.89727	0.563681
F21	-2.66988	-2.62547	-0.2466
F22	-3.23635	0.568693	3.198005
F23	-5.48855	-0.71663	4.011927
C31	0.822871	-2.13735	5.111756
C32	0.237749	-2.87135	4.082659
C33	-0.25479	-2.21759	2.958446
C34	-0.19707	-0.81913	2.84945
C35	0.414947	-0.10677	3.891175

C36	0.917138	-0.75004	5.014753
F30	1.291201	-2.76236	6.190315
F31	0.158238	-4.20002	4.174552
F32	-0.78554	-2.95154	1.976308
F33	0.518458	1.222458	3.802141
F34	1.478563	-0.04957	6.001381
C42	-4.44563	0.216719	-3.27579
C43	-4.7029	0.946041	-2.11782
C44	-3.75054	0.973047	-1.10628
C45	-2.5381	0.279842	-1.2039
C46	-2.31055	-0.45307	-2.37474
C47	-3.24734	-0.48123	-3.40365
F41	-5.34736	0.179652	-4.25548
F42	-5.85172	1.611362	-1.98341
F43	-4.00404	1.680765	0.009208
F44	-1.18187	-1.1517	-2.5284
F45	-3.00703	-1.18983	-4.50751
O53	0.607424	2.612376	0.607027
C54	-0.34269	3.343355	0.884786
O55	-1.60238	3.037845	0.833833
C56	-0.08543	4.804655	1.322648
F57	-0.7665	5.072494	2.442975
F58	1.212545	5.002008	1.537817
F59	-0.50267	5.629287	0.35179
O60	0.611938	-1.43977	-0.28649
C61	1.616863	-1.95688	-0.93363
O62	2.546719	-1.39516	-1.48233
C63	1.481759	-3.50629	-0.95468
F64	2.542694	-4.07215	-1.53532
F65	1.375339	-3.99343	0.298504
F66	0.379139	-3.87239	-1.63759
H67	2.033592	1.385766	-1.18916
C62	1.061191	1.10484	-2.1182
H62	0.725368	0.126818	-2.44212
H64	1.888236	1.396987	-2.77856
O64	-0.03923	2.025588	-2.32243
C65	0.192201	3.175511	-2.96418
O66	1.236869	3.574337	-3.40616
C67	-1.13967	3.953773	-3.06512
F68	-1.64622	4.173111	-1.8301

F69	-0.95735	5.125735	-3.66428
F70	-2.04915	3.244237	-3.75945

Table S64. [$Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_2OH^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.406656	0.586521	-0.3461
N2	-0.5701	0.243846	1.474616
C3	3.409742	0.98928	-0.08998
O4	3.753627	0.036277	-0.79751
C5	-1.65207	-0.27031	0.875032
O6	2.248949	1.36011	0.289769
N7	-1.5453	-0.09488	-0.43622
C8	0.316417	1.346776	-3.05766
O9	1.076667	0.627138	-2.34721
O10	-0.58431	2.101726	-2.62047
C11	0.448991	1.217174	-4.59027
F12	-0.559	0.436135	-5.03533
F13	0.346401	2.413774	-5.17919
F14	1.606591	0.657222	-4.94717
C15	4.522134	1.90581	0.488204
F16	4.175868	3.205596	0.347585
F17	4.675451	1.660327	1.803258
F18	5.69274	1.716023	-0.11903
H19	-0.36653	2.016197	-1.21111
C20	-4.87807	-2.21474	2.922867
C21	-4.30594	-2.81477	1.80268
C22	-3.26248	-2.17795	1.139998
C23	-2.77537	-0.93736	1.569674
C24	-3.36712	-0.3571	2.697561
C25	-4.40874	-0.98226	3.373758
F26	-5.87352	-2.82011	3.564014
F27	-4.75097	-3.99803	1.378901
F28	-2.71917	-2.78938	0.083651
F29	-2.94164	0.829777	3.145358
F30	-4.96078	-0.40777	4.443199
C31	1.150552	-0.81279	5.172022
C32	0.609389	-1.80835	4.362785
C33	0.030535	-1.47123	3.144203
C34	-0.05133	-0.1372	2.710131
C35	0.513103	0.840497	3.543968

C36	1.107192	0.516745	4.757497
F37	1.710177	-1.13048	6.338934
F38	0.659511	-3.08504	4.751316
F39	-0.44754	-2.45941	2.375546
F40	0.482364	2.126085	3.170061
F41	1.625815	1.471681	5.531738
C42	-4.43965	-0.41079	-3.46901
C43	-4.74994	0.253958	-2.28503
C44	-3.79642	0.349898	-1.27873
C45	-2.52961	-0.23755	-1.40731
C46	-2.24566	-0.89884	-2.60891
C47	-3.17875	-0.97979	-3.63508
F48	-5.34655	-0.49941	-4.44176
F49	-5.95257	0.812273	-2.12606
F50	-4.09759	1.039325	-0.16611
F51	-1.03507	-1.44184	-2.79373
F52	-2.87603	-1.60793	-4.77098
O53	0.867961	-1.5686	-0.20089
C54	1.491342	-2.2858	-0.99141
O55	2.564363	-2.00337	-1.63676
C56	0.978294	-3.72801	-1.22008
F57	1.225684	-4.13761	-2.46745
F58	1.599435	-4.5565	-0.36174
F59	-0.33923	-3.79444	-0.99645
H60	2.966018	-1.08906	-1.34023
C61	-0.09647	2.826903	-0.07517
H62	-1.04994	3.260639	-0.39685
H63	-0.13185	2.628431	0.993267
O64	0.936516	3.623483	-0.50129
H65	1.748249	3.296639	-0.07723

Table S65. [$Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_2OH^{eq}$-H-$TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.492177	0.461701	-0.09989
N2	-0.42306	-0.20467	1.707099
C3	3.525268	0.638372	0.38861
O4	3.90945	-0.31331	-0.31807
C5	-1.56738	-0.46728	1.093572
O6	2.359075	1.082878	0.598562
N7	-1.51092	-0.09853	-0.18961

C8	4.615732	1.44644	1.146147
F9	4.569634	2.739826	0.780863
F10	4.400104	1.37398	2.472305
F11	5.841337	0.979672	0.891947
H12	0.193778	1.60635	-1.79796
C13	-4.96053	-2.34102	2.922894
C14	-4.46	-2.83406	1.718555
C15	-3.36215	-2.21703	1.129228
C16	-2.74716	-1.10729	1.72075
C17	-3.26536	-0.63402	2.930599
C18	-4.36409	-1.23846	3.532264
F19	-6.01019	-2.92629	3.493597
F20	-5.02813	-3.89611	1.145137
F21	-2.88973	-2.71878	-0.01617
F22	-2.71235	0.422887	3.531834
F23	-4.84906	-0.76675	4.681632
C24	1.286439	-2.02868	5.085005
C25	0.639801	-2.81727	4.136219
C26	0.056205	-2.21841	3.026517
C27	0.076656	-0.8256	2.844456
C28	0.746378	-0.05642	3.80914
C29	1.345244	-0.64655	4.917089
F30	1.849809	-2.59659	6.152086
F31	0.593386	-4.14419	4.287763
F32	-0.52306	-3.00511	2.10641
F33	0.815279	1.265869	3.66455
F34	1.968214	0.104821	5.827555
C35	-4.78269	0.714288	-2.72042
C36	-4.72031	1.295111	-1.45582
C37	-3.6411	1.019864	-0.62363
C38	-2.60842	0.149997	-1.00898
C39	-2.70333	-0.41543	-2.28749
C40	-3.76571	-0.14085	-3.13971
F41	-5.80999	0.975779	-3.52776
F42	-5.68524	2.124553	-1.05512
F43	-3.58396	1.613716	0.576748
F44	-1.74026	-1.24984	-2.72128
F45	-3.82243	-0.70258	-4.34889
O46	-0.11192	2.373966	0.386267
C47	-0.60412	3.005467	-0.58278

O48	-0.58387	2.622964	-1.78652
C49	-1.33583	4.331709	-0.28962
F50	-2.64852	4.154856	-0.53473
F51	-1.18228	4.71269	0.976654
F52	-0.87825	5.296326	-1.09731
O53	0.76089	-1.61603	-0.35429
C54	1.508971	-2.39146	-0.96801
O55	2.736757	-2.24982	-1.27895
C56	0.880883	-3.75578	-1.33943
F57	1.61376	-4.41265	-2.2394
F58	0.784491	-4.50533	-0.22652
F59	-0.35079	-3.56942	-1.83367
H60	3.167327	-1.35901	-0.89183
C61	1.256621	0.757114	-2.28396
H62	1.243299	1.621183	-2.97373
H63	2.284889	0.70295	-1.93315
O64	0.963275	-0.43655	-2.96098
H65	0.019462	-0.47996	-3.16224

Table S66. [$Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_2OH^{eq}$-H-$TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.4782	0.327801	-0.11109
N2	-0.526	-0.31297	1.66285
C3	3.541335	0.998305	0.134769
O4	4.029291	0.236538	-0.76903
C5	-1.63619	-0.56765	0.980553
O6	2.392365	1.011367	0.601956
N7	-1.47149	-0.24353	-0.30027
C8	4.562345	2.004721	0.720622
F9	3.933547	3.044468	1.275791
F10	5.293958	1.387578	1.663555
F11	5.382937	2.454712	-0.23474
H12	1.137285	1.701766	-1.46387
C13	-5.28266	-2.07645	2.655187
C14	-4.74479	-2.67818	1.518488
C15	-3.56023	-2.18926	0.978914
C16	-2.89333	-1.10163	1.55346
C17	-3.45	-0.51888	2.697787
C18	-4.63556	-0.99413	3.248178
F19	-6.41622	-2.53874	3.176641

F20	-5.36192	-3.72153	0.961532
F21	-3.05743	-2.7948	-0.10106
F22	-2.85306	0.522921	3.283006
F23	-5.15518	-0.41661	4.33261
C24	1.012436	-2.20225	5.085793
C25	0.319727	-2.95677	4.142288
C26	-0.20946	-2.33657	3.016786
C27	-0.09253	-0.95054	2.814389
C28	0.623945	-0.21861	3.774651
C29	1.171598	-0.83086	4.896128
F30	1.526135	-2.79236	6.166735
F31	0.180371	-4.27477	4.313086
F32	-0.83027	-3.09607	2.102701
F33	0.797854	1.093936	3.603938
F34	1.84307	-0.11006	5.798523
C35	-4.3639	0.29629	-3.2965
C36	-4.46837	1.006584	-2.10249
C37	-3.51121	0.824096	-1.11092
C38	-2.45077	-0.07811	-1.27395
C39	-2.36993	-0.7802	-2.48432
C40	-3.30989	-0.59508	-3.49034
F41	-5.27572	0.466919	-4.25446
F42	-5.4775	1.863647	-1.92004
F43	-3.61191	1.524378	0.026998
F44	-1.36927	-1.64201	-2.68339
F45	-3.21803	-1.27263	-4.6367
O46	-0.16917	2.263248	0.342182
C47	0.376847	3.160461	-0.33897
O48	1.172077	2.957004	-1.30719
C49	0.024847	4.630217	-0.02775
F50	1.116508	5.398201	-0.1163
F51	-0.87328	5.054598	-0.93679
F52	-0.50146	4.758225	1.18947
O53	0.858125	-1.69563	-0.30761
C54	1.82537	-2.30342	-0.85046
O55	2.886714	-1.85081	-1.32193
C56	1.582669	-3.8352	-0.9318
F57	2.644001	-4.47721	-1.42551
F58	1.318127	-4.32435	0.29322
F59	0.524932	-4.0833	-1.72387

H60	3.424918	-0.61658	-1.02711
C61	0.928845	0.609486	-2.37638
H62	0.80748	-0.46594	-2.45049
H63	1.93144	0.848527	-2.76856
O64	-0.10777	1.188781	-3.13062
H65	0.054544	2.140304	-3.19715

Table S67. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})(CH_2OH^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.609802	0.555247	0.074586
N2	-0.58161	-0.0907	1.740874
C3	3.405347	0.9999	0.339775
O4	3.291106	1.566094	-0.7757
C5	-1.66565	-0.24179	1.019619
O6	2.475155	0.419117	0.961918
N7	-1.5641	0.427407	-0.16117
C8	4.787853	1.057595	1.02394
F9	5.75186	0.758383	0.147037
F10	4.993418	2.306665	1.479192
F11	4.861928	0.211065	2.054756
H12	-1.6113	2.099491	0.299986
C13	-5.12257	-2.44757	2.268607
C14	-4.34643	-2.92448	1.212611
C15	-3.22765	-2.20494	0.805165
C16	-2.86807	-1.01115	1.43608
C17	-3.65885	-0.55415	2.492109
C18	-4.78244	-1.25831	2.911933
F19	-6.19357	-3.13077	2.664716
F20	-4.67514	-4.0656	0.606252
F21	-2.48578	-2.68116	-0.19703
F22	-3.33823	0.585912	3.115425
F23	-5.53208	-0.80403	3.917345
C24	0.701272	-1.98935	5.260559
C25	0.220245	-2.7655	4.208784
C26	-0.23921	-2.15235	3.047721
C27	-0.24664	-0.75527	2.918536
C28	0.260553	0.000754	3.984999
C29	0.725249	-0.60032	5.14773
F30	1.138047	-2.57504	6.375428
F31	0.209187	-4.0963	4.314286

F32	-0.66381	-2.92546	2.043289
F33	0.299907	1.33344	3.882157
F34	1.187926	0.142921	6.155501
C35	-4.51348	0.098817	-3.18676
C36	-4.74975	0.856661	-2.04249
C37	-3.76566	0.938277	-1.06482
C38	-2.53777	0.271898	-1.17889
C39	-2.33513	-0.49326	-2.33407
C40	-3.30337	-0.57393	-3.33221
F41	-5.4445	0.01446	-4.13671
F42	-5.91014	1.498849	-1.89032
F43	-4.00728	1.669564	0.036366
F44	-1.19659	-1.17037	-2.51229
F45	-3.0792	-1.3084	-4.42285
O46	0.689349	2.608728	0.691539
C47	-0.28544	3.345932	0.843057
O48	-1.52766	3.055714	0.622523
C49	-0.08257	4.789139	1.358382
F50	-0.7093	4.938125	2.532849
F51	1.213914	5.050658	1.517389
F52	-0.5997	5.658002	0.478494
O53	0.611824	-1.41143	-0.32393
C54	1.525743	-1.93127	-1.08703
O55	2.442988	-1.38272	-1.67178
C56	1.297727	-3.46532	-1.19625
F57	2.22093	-4.03677	-1.9753
F58	1.355772	-4.0428	0.02073
F59	0.083189	-3.72572	-1.721
H60	2.088166	1.23599	-1.17263
C61	1.031263	1.209659	-2.08352
H62	0.285226	0.479824	-2.37987
H63	1.89429	1.019628	-2.74114
O64	0.497269	2.50168	-2.23596
H65	1.219534	3.137756	-2.14115

Rh(NN^F) complexes in H_2O

Table S68. [Rh^I(NN^F)(OH)(H_2O)]$^-$·4H_2O

Atom	x	y	z

Rh1	0.291802	0.081188	-0.15615
N2	-0.85666	-0.01011	1.619554
H3	3.263751	0.046454	0.55581
C4	-1.89819	-0.60726	1.009095
O5	2.065103	1.135538	0.362602
N6	-1.57318	-0.83205	-0.26532
H7	1.982972	-0.22659	-2.19876
C8	-5.72576	-1.49181	2.77881
C9	-5.08304	-2.43848	1.986873
C10	-3.84234	-2.14738	1.431909
C11	-3.20991	-0.9104	1.623538
C12	-3.88881	0.023363	2.420424
C13	-5.1219	-0.25763	2.998848
F14	-6.91852	-1.76666	3.325172
F15	-5.65382	-3.63586	1.785211
F16	-3.24628	-3.10955	0.713937
F17	-3.37021	1.241068	2.635573
F18	-5.74526	0.662843	3.750439
C19	-0.01817	0.279404	5.751308
C20	-0.65988	-0.85057	5.25734
C21	-0.94491	-0.96126	3.901342
C22	-0.63887	0.058371	2.971607
C23	0.031365	1.175988	3.514447
C24	0.337265	1.290312	4.863055
F25	0.257461	0.392787	7.06297
F26	-0.98025	-1.85151	6.095811
F27	-1.4955	-2.11719	3.480931
F28	0.394693	2.192157	2.706492
F29	0.958961	2.389681	5.323161
C30	-4.08263	-1.60544	-3.56167
C31	-4.4404	-0.62562	-2.64261
C32	-3.62861	-0.37732	-1.5413
C33	-2.44939	-1.10534	-1.29878
C34	-2.11089	-2.08162	-2.25452
C35	-2.90954	-2.32857	-3.36516
F36	-4.86424	-1.85555	-4.6265
F37	-5.56237	0.090994	-2.83289
F38	-3.98915	0.617419	-0.70922
F39	-1.00659	-2.8133	-2.09585
F40	-2.56632	-3.28127	-4.24787

O41	0.996947	-0.10775	-2.17793
H42	0.851353	0.759145	-2.62126
H43	1.78944	1.619681	1.151019
O44	2.990442	2.532559	-1.47727
O45	1.148381	2.373614	-3.42149
O46	3.72218	-0.05899	-2.22515
O47	4.08483	-0.52964	0.468011
H48	2.558667	2.006525	-0.66253
H49	3.387683	3.3358	-1.12289
H50	1.777921	2.603622	-2.69214
H51	1.7303	2.079551	-4.13405
H52	3.926752	-0.40489	-1.324
H53	3.710958	0.907485	-2.08029
H54	4.810174	0.075087	0.668851

Table S69. $Rh^{I}(NN^{F})(H_2O)_2 \cdot 4H_2O$

Atom	x	y	z
Rh1	0.442141	0.206195	-0.26262
N2	-0.58902	-0.22263	1.527758
H3	2.624347	0.630286	1.019943
C4	-1.58366	-0.84409	0.899036
O5	2.257406	1.204883	0.313691
N6	-1.37785	-0.85131	-0.41525
H7	0.333496	0.872509	-2.73861
C8	-4.99518	-2.57213	2.856655
C9	-4.16993	-3.36979	2.066232
C10	-3.0682	-2.80072	1.435379
C11	-2.76564	-1.443	1.57503
C12	-3.61012	-0.66542	2.373545
C13	-4.71687	-1.21541	3.012445
F14	-6.05264	-3.10764	3.464521
F15	-4.43564	-4.67075	1.925814
F16	-2.28637	-3.58912	0.688076
F17	-3.3686	0.641698	2.532149
F18	-5.51489	-0.4536	3.76448
C19	0.260469	-0.48981	5.652565
C20	0.279816	-1.63458	4.859701
C21	-0.02729	-1.53748	3.507749
C22	-0.3677	-0.31843	2.902819
C23	-0.38517	0.809643	3.732159

C24	-0.07307	0.737267	5.085176
F25	0.554643	-0.56857	6.952301
F26	0.605228	-2.81381	5.397419
F27	0.028066	-2.64543	2.749575
F28	-0.73712	2.010152	3.228327
F29	-0.11013	1.835898	5.845336
C30	-4.28404	-1.67172	-3.36192
C31	-4.45639	-0.59927	-2.49018
C32	-3.5051	-0.35519	-1.50729
C33	-2.36741	-1.15961	-1.34993
C34	-2.23071	-2.23317	-2.23821
C35	-3.16535	-2.49154	-3.23494
F36	-5.18945	-1.91695	-4.31192
F37	-5.52464	0.194313	-2.61121
F38	-3.66863	0.702842	-0.6956
F39	-1.17859	-3.0696	-2.1262
F40	-3.00349	-3.53214	-4.05808
O41	1.124205	0.51723	-2.27824
H42	1.309552	-0.39329	-2.60651
H43	1.943558	2.04987	0.712389
O44	0.629832	3.239707	0.995743
O45	-1.29218	1.721656	-2.71539
O46	1.559975	-2.14147	-2.27494
O47	2.756512	-0.99664	1.854726
H48	0.092613	2.633051	0.451087
H49	0.27726	3.09658	1.886011
H50	-1.34849	1.549263	-1.75857
H51	-1.13996	2.674045	-2.78482
H52	0.741718	-2.61458	-2.48468
H53	1.427221	-1.88411	-1.3424
H54	3.464256	-1.49998	1.429461
H55	1.944273	-1.274	1.393853

Table S70. $[Rh^{III}(NN^{F})(OH)_3(H_2O^{ax})]^{-}\cdot 8H_2O$

Atom	x	y	z
Rh1	0.19546	0.231968	-0.05015
N2	-0.90159	-0.2977	1.698657
H3	4.967458	0.304722	-0.84396
C4	-1.85479	-0.92518	1.020341
O5	1.864445	1.255204	0.5806

N6	-1.6609	-0.81472	-0.29243
H7	1.656032	2.311259	-2.45493
C8	-5.08278	-3.07057	2.896939
C9	-4.35184	-3.66823	1.874223
C10	-3.31363	-2.96622	1.268824
C11	-2.9802	-1.66592	1.659159
C12	-3.7333	-1.08999	2.686993
C13	-4.77336	-1.77631	3.305559
F14	-6.08154	-3.73796	3.48522
F15	-4.64562	-4.91612	1.486554
F16	-2.62926	-3.58164	0.300322
F17	-3.47978	0.156987	3.099324
F18	-5.48389	-1.19755	4.282763
C19	0.537499	-0.98343	5.595449
C20	0.159085	-2.06386	4.806437
C21	-0.33706	-1.85144	3.524772
C22	-0.49698	-0.55976	2.993381
C23	-0.09653	0.50702	3.815116
C24	0.413557	0.308125	5.091109
F25	1.0117	-1.1826	6.834298
F26	0.285608	-3.31157	5.282133
F27	-0.65523	-2.92804	2.791921
F28	-0.21914	1.769356	3.370796
F29	0.768847	1.356037	5.8503
C30	-4.46201	-1.13198	-3.43011
C31	-4.85109	-0.58397	-2.21322
C32	-3.93752	-0.48055	-1.17102
C33	-2.61336	-0.94677	-1.2816
C34	-2.25063	-1.46935	-2.53609
C35	-3.14948	-1.56548	-3.59072
F36	-5.34044	-1.23855	-4.43821
F37	-6.10659	-0.13727	-2.05449
F38	-4.34884	0.119233	-0.03981
F39	-0.99225	-1.88563	-2.74786
F40	-2.76156	-2.0902	-4.7618
O41	1.017705	0.631303	-1.87141
H42	1.600253	-0.10456	-2.13413
H43	2.25191	1.339402	-0.30918
O44	2.147941	5.031563	-0.76105
O45	1.682024	3.191195	-2.88774

O46	3.08054	-1.29728	-2.60404
O47	4.993299	-0.65603	-0.75719
H48	3.068505	4.808238	-0.57664
H49	1.653249	4.638286	-0.0057
H50	1.780401	3.845254	-2.16621
H51	2.514766	-2.09851	-2.34379
H52	3.30842	-1.40795	-3.53402
H53	4.340364	-0.96516	-1.4289
O54	-0.96031	2.067809	-0.28119
O55	1.105824	-1.54191	0.182852
H56	-0.42417	2.772773	0.149184
H57	-0.99152	2.247194	-1.26939
O58	-0.87506	2.168318	-2.92765
H59	-0.30995	1.369237	-2.78339
H60	-0.16127	2.820128	-3.10732
O61	0.891565	3.52352	1.092585
H62	1.363738	2.611168	0.95142
H63	0.623732	3.538183	2.019522
H64	1.919376	-1.39087	0.712074
O65	3.415884	-0.76284	1.61588
H66	2.947124	0.073921	1.405207
H67	4.050742	-0.85095	0.876141
O68	1.508359	-3.1515	-1.74445
H69	0.670701	-3.09928	-2.22221
H70	1.331282	-2.55509	-0.923

Table S71. $[Rh^{III}(NN^{F})(OH)_3(H_2O^{eq})]^{-}\cdot 8H_2O$

Atom	x	y	z
Rh1	0.318968	-0.02067	-0.11318
N2	-0.84357	-0.14427	1.61028
H3	3.393182	0.058468	0.689389
C4	-1.90356	-0.66768	0.993114
O5	2.050707	0.920693	0.44857
N6	-1.63119	-0.87294	-0.29276
H7	2.151357	-0.25699	-1.98441
C8	-5.70758	-1.47775	2.829126
C9	-5.08428	-2.45433	2.057047
C10	-3.85227	-2.18377	1.470676
C11	-3.21498	-0.95031	1.637243
C12	-3.86514	0.012753	2.41493

C13	-5.0974	-0.23948	3.009938
F14	-6.89145	-1.72844	3.395411
F15	-5.66822	-3.64673	1.890592
F16	-3.27832	-3.14905	0.746618
F17	-3.31845	1.219745	2.59434
F18	-5.70366	0.70189	3.742795
C19	0.262851	-0.34074	5.667748
C20	-0.40607	-1.41125	5.087215
C21	-0.78574	-1.34915	3.752849
C22	-0.54484	-0.21516	2.962206
C23	0.151299	0.836332	3.574316
C24	0.551657	0.783702	4.901212
F25	0.625683	-0.39027	6.956825
F26	-0.67097	-2.50696	5.813034
F27	-1.37007	-2.43468	3.212829
F28	0.461259	1.930469	2.85685
F29	1.202837	1.815929	5.454046
C30	-4.29633	-0.96981	-3.54646
C31	-4.48171	-0.03128	-2.53674
C32	-3.61406	-0.00852	-1.45142
C33	-2.55935	-0.92606	-1.32131
C34	-2.38845	-1.85101	-2.36389
C35	-3.24225	-1.87576	-3.46132
F36	-5.12954	-1.00322	-4.59564
F37	-5.4852	0.853117	-2.62124
F38	-3.79435	0.941213	-0.51497
F39	-1.39122	-2.73503	-2.30467
F40	-3.06968	-2.78022	-4.43422
O41	1.153217	-0.2004	-2.05008
H42	1.013318	0.614453	-2.59585
H43	1.809732	1.370879	1.269841
O44	2.757012	2.739016	-1.36794
O45	1.392345	2.05604	-3.49689
O46	3.830898	0.097108	-2.01914
O47	4.310236	-0.35966	0.682334
H48	2.469182	2.071056	-0.67847
H49	2.184428	3.518179	-1.13289
H50	1.95133	2.374651	-2.71668
H51	2.017602	1.830566	-4.19668
H52	4.135124	-0.23406	-1.14283

H53	3.81586	1.061825	-1.90505
H54	4.89566	0.358607	0.955721
O55	1.168809	-1.83126	0.344185
O56	-0.49813	1.839968	-0.56332
H57	0.432192	-2.45775	0.387207
H58	-1.26197	1.9352	0.021794
H59	3.285495	-1.21648	2.391342
O60	2.40168	-1.38654	2.749338
H61	1.917306	-1.63627	1.926125
H62	1.183013	-2.43406	-2.5728
O63	1.638556	-3.1368	-2.09248
H64	1.682179	-2.74093	-1.19733
H65	-0.22339	3.101989	-3.32633
O66	-0.94201	3.444611	-2.76747
H67	-0.95887	2.769269	-2.04939
H68	0.342633	3.427785	-0.35088
O69	0.702389	4.298716	-0.65132
H70	0.184423	4.386623	-1.47893

Table S72. $Rh^{III}(NN^{F})(OH)_2(H_2O^{ax})_2 \cdot 8H_2O$

Atom	x	y	z
Rh1	0.183098	0.122686	-0.14814
N2	-0.77318	-0.37132	1.6242
H3	2.209477	1.007728	1.305876
C4	-1.79502	-0.96307	1.008939
O5	1.935729	1.19334	0.37398
N6	-1.61221	-0.9085	-0.30828
H7	0.170307	0.363016	-2.78199
C8	-5.16339	-2.74642	2.978693
C9	-4.45807	-3.46913	2.017899
C10	-3.36883	-2.88248	1.382561
C11	-2.95994	-1.57976	1.687952
C12	-3.68424	-0.87606	2.656797
C13	-4.77803	-1.44595	3.300186
F14	-6.20774	-3.29955	3.590685
F15	-4.82428	-4.71691	1.719402
F16	-2.70315	-3.60042	0.47313
F17	-3.34157	0.375629	2.977009
F18	-5.46115	-0.75442	4.214152
C19	0.569937	-1.07842	5.548324

C20	0.250055	-2.15394	4.723157
C21	-0.19643	-1.90953	3.431646
C22	-0.36755	-0.60926	2.9352
C23	-0.01755	0.45225	3.779361
C24	0.445567	0.224068	5.07112
F25	1.002971	-1.29742	6.791549
F26	0.389923	-3.40679	5.168112
F27	-0.44015	-2.95957	2.620094
F28	-0.11689	1.705615	3.340065
F29	0.766453	1.251703	5.8619
C30	-4.5788	-1.14198	-3.28254
C31	-4.75981	-0.29603	-2.19084
C32	-3.77691	-0.23183	-1.21274
C33	-2.61413	-1.01245	-1.27142
C34	-2.44959	-1.83976	-2.3895
C35	-3.41929	-1.90652	-3.3851
F36	-5.51424	-1.21467	-4.23156
F37	-5.86208	0.454581	-2.09863
F38	-3.93452	0.632753	-0.18845
F39	-1.34603	-2.57462	-2.51222
F40	-3.24805	-2.71063	-4.43793
O41	0.900863	0.430499	-2.1193
H42	1.689393	-0.17321	-2.38507
H43	1.879722	2.207061	0.209207
O44	1.805471	3.713631	-0.06927
O45	-1.15233	1.041031	-3.74125
O46	2.890609	-1.05199	-2.7631
O47	3.090956	0.087812	2.532001
H48	1.37798	3.799295	-0.94305
H49	1.094012	3.983688	0.568215
H50	-0.90409	1.947177	-3.44814
H51	-0.99364	1.026549	-4.69369
H52	2.472768	-1.95208	-2.73892
H53	3.476354	-1.04763	-1.9817
H54	3.791398	0.589795	2.9678
H55	3.540092	-0.43148	1.826965
O56	-0.85576	1.914818	-0.24497
O57	1.238897	-1.6595	-0.06014
H58	-1.79733	1.69439	-0.25541
H59	0.893306	-2.15311	0.6962

O60	3.766229	-0.88625	0.005411
O61	1.476357	-3.25051	-2.21064
H62	3.515647	0.042585	-0.14302
H63	2.858031	-1.30742	0.031079
H64	1.244081	-2.74251	-1.38835
H65	1.992895	-4.0075	-1.90791
O66	-0.36737	3.917633	1.475176
O67	0.137974	3.109533	-2.37991
H68	-0.6513	3.117493	0.958127
H69	-0.98231	4.617565	1.223212
H70	0.819755	2.423237	-2.48692
H71	-0.34708	2.747667	-1.58146

Table S73. $Rh^{III}(NN^{F})(OH)_2(H_2O^{ax})(H_2O^{eq})\cdot 8H_2O$

Atom	x	y	z
Rh1	0.271388	0.157706	-0.13082
N2	-0.893	0.03319	1.582559
H3	3.543394	0.279617	-0.06141
C4	-1.9274	-0.53595	0.960172
O5	2.004905	1.117579	0.503742
N6	-1.6342	-0.73451	-0.31924
H7	1.894596	-0.44959	-2.21926
C8	-5.64581	-1.54326	2.856609
C9	-4.98578	-2.48994	2.075687
C10	-3.77909	-2.15684	1.469136
C11	-3.20893	-0.88848	1.620142
C12	-3.89106	0.042311	2.412437
C13	-5.09833	-0.27309	3.026806
F14	-6.80128	-1.85252	3.441011
F15	-5.50752	-3.7083	1.920165
F16	-3.1622	-3.09011	0.73584
F17	-3.39914	1.273486	2.585084
F18	-5.73613	0.633921	3.769958
C19	0.040113	-0.17722	5.681734
C20	-0.27681	-1.33925	4.982332
C21	-0.59559	-1.25919	3.632584
C22	-0.63204	-0.03632	2.946637
C23	-0.30754	1.112421	3.678591
C24	0.028461	1.051287	5.025614
F25	0.349268	-0.23898	6.978046

F26	-0.26004	-2.52005	5.605906
F27	-0.86863	-2.39401	2.962718
F28	-0.33733	2.314577	3.079815
F29	0.321131	2.168295	5.698797
C30	-4.20131	-1.35095	-3.59528
C31	-4.5142	-0.37496	-2.65342
C32	-3.67896	-0.17704	-1.55965
C33	-2.52696	-0.95341	-1.36042
C34	-2.23747	-1.92631	-2.32788
C35	-3.05506	-2.12606	-3.43336
F36	-4.99841	-1.54583	-4.64849
F37	-5.60802	0.378258	-2.81012
F38	-3.98803	0.794258	-0.68684
F39	-1.15596	-2.7047	-2.17997
F40	-2.75829	-3.06982	-4.3317
O41	1.013358	0.063309	-2.09858
H42	1.197399	0.949614	-2.48648
H43	2.286085	0.603582	1.301504
O44	3.0992	3.071772	-1.03559
O45	1.742854	2.486698	-3.18105
O46	3.212613	-1.17276	-2.53056
O47	4.372998	-0.2322	-0.19978
H48	2.851779	2.276209	-0.50484
H49	2.66702	3.780351	-0.53093
H50	2.304841	2.807504	-2.40863
H51	2.341168	2.295498	-3.91371
H52	2.874669	-2.08792	-2.35088
H53	3.798631	-0.9643	-1.77252
H54	5.067758	0.430707	-0.30374
O55	1.106547	-1.64003	0.318673
O56	-0.67834	2.038121	-0.48972
H57	0.402045	-2.1543	0.739986
H58	3.697509	-0.90065	1.80317
O59	2.82844	-0.81729	2.226406
H60	2.233421	-1.30353	1.601154
H61	1.050995	-3.3232	-2.25951
O62	1.839595	-3.30592	-1.70186
H63	1.570648	-2.74124	-0.93309
H64	0.038234	2.880785	-3.26655
O65	-0.90776	2.894778	-2.99956

H66	-0.7987	2.319681	-1.43801
H67	-0.15068	2.737785	-0.02446
O68	1.067599	3.530041	0.869794
H69	1.469694	2.613961	0.95203
H70	0.744066	3.755445	1.75106
H71	-1.18641	3.817899	-3.03419

Table S74. $Rh^{III}(NN^{F})(OH)_2(H_2O^{eq})_2 \cdot 8H_2O$

Atom	x	y	z
Rh1	0.208293	0.147141	-0.10911
N2	-0.82265	-0.33	1.653795
H3	5.92166	-0.42067	0.205798
C4	-1.82065	-0.93375	1.016735
O5	1.879126	1.154872	0.584817
N6	-1.62414	-0.88702	-0.29994
H7	0.686124	1.759351	-3.04826
C8	-5.18135	-2.78832	2.946339
C9	-4.47187	-3.4807	1.967512
C10	-3.38685	-2.8712	1.346325
C11	-2.98538	-1.57343	1.680319
C12	-3.7152	-0.9013	2.666489
C13	-4.80349	-1.49441	3.297926
F14	-6.22217	-3.36395	3.546294
F15	-4.83018	-4.72416	1.637635
F16	-2.71932	-3.56674	0.41986
F17	-3.38571	0.344954	3.019413
F18	-5.48964	-0.82899	4.230537
C19	0.542622	-0.85386	5.600535
C20	0.140775	-1.96196	4.860717
C21	-0.32675	-1.79428	3.562243
C22	-0.43321	-0.52461	2.971268
C23	-0.01373	0.570256	3.74106
C24	0.470912	0.41623	5.033666
F25	0.994441	-1.00696	6.848054
F26	0.221449	-3.18536	5.393872
F27	-0.66358	-2.88729	2.86212
F28	-0.08138	1.807924	3.225647
F29	0.855092	1.484519	5.741964
C30	-4.44249	-1.3005	-3.40382
C31	-4.7664	-0.55201	-2.27564

C32	-3.84396	-0.42045	-1.24238
C33	-2.58563	-1.04534	-1.28473
C34	-2.29034	-1.78726	-2.43882
C35	-3.19488	-1.91451	-3.4859
F36	-5.32096	-1.42751	-4.40201
F37	-5.95552	0.054986	-2.19677
F38	-4.17485	0.342641	-0.18989
F39	-1.10468	-2.40732	-2.54116
F40	-2.87918	-2.63778	-4.56585
O41	0.929651	0.339888	-2.04377
H42	1.880465	0.529092	-1.95823
H43	2.352178	1.513465	-0.18494
O44	2.337144	3.53867	-1.32024
O45	0.65405	2.672787	-3.42451
O46	3.910239	-0.45522	-2.26592
O47	5.336891	-1.15752	-0.0082
H48	3.049106	4.183851	-1.4035
H49	1.829041	3.802515	-0.52411
H50	1.256511	3.156543	-2.82511
H51	3.302848	-1.19686	-2.49296
H52	4.347701	-0.21398	-3.09154
H53	4.912582	-0.91325	-0.86004
O54	-0.90602	1.913303	-0.13665
O55	1.151114	-1.70368	0.093135
H56	-0.387	2.622409	0.318147
H57	-1.21433	2.285599	-1.02525
O58	-1.68199	3.050842	-2.32956
H59	-2.34724	2.57946	-2.84506
H60	-0.83483	3.013653	-2.86947
O61	0.934294	3.473539	1.026589
H62	1.364146	2.552819	1.083592
H63	0.797194	3.796242	1.924976
H64	1.985809	-1.56467	0.677728
H65	1.421605	-2.02047	-0.80111
O66	3.103347	-1.02507	1.574846
H67	2.830733	-0.0984	1.367736
H68	3.963591	-1.14886	1.109778
O69	1.740851	-2.01711	-2.54272
H70	1.234442	-1.1347	-2.52487
H71	1.242887	-2.64072	-3.08384

Table S75. $[Rh^{III}(NN^{F})(OH)_2(H_2O^{ax})(CH_3^{ax})]^{-}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.141956	0.376408	-0.06505
N2	-0.82872	-0.29976	1.702677
H3	3.780018	-0.91626	-0.86643
C4	-1.80626	-0.91974	1.045166
O5	1.72119	1.463435	0.672955
N6	-1.64308	-0.79988	-0.26804
H7	2.192902	1.585319	-1.96829
C8	-5.02055	-3.06871	2.942318
C9	-4.24676	-3.68946	1.966344
C10	-3.21082	-2.98534	1.360656
C11	-2.92297	-1.66069	1.701356
C12	-3.71548	-1.06319	2.685693
C13	-4.75438	-1.75161	3.305081
F14	-6.01759	-3.7377	3.532418
F15	-4.49535	-4.96122	1.626458
F16	-2.47768	-3.62327	0.441654
F17	-3.49922	0.204281	3.053333
F18	-5.50488	-1.15386	4.240219
C19	0.420964	-0.72815	5.701027
C20	0.083191	-1.85717	4.963457
C21	-0.34446	-1.72239	3.647519
C22	-0.47899	-0.46806	3.025771
C23	-0.1133	0.651647	3.795738
C24	0.328839	0.528047	5.107503
F25	0.832572	-0.84774	6.973296
F26	0.191665	-3.07536	5.518159
F27	-0.6017	-2.84662	2.95293
F28	-0.20542	1.877373	3.270465
F29	0.649897	1.619834	5.819266
C30	-4.3743	-1.42944	-3.4105
C31	-4.81262	-0.82788	-2.23668
C32	-3.9253	-0.62544	-1.18551
C33	-2.58282	-1.03727	-1.25211
C34	-2.16876	-1.62707	-2.46056
C35	-3.04322	-1.8217	-3.52268
F36	-5.22793	-1.63197	-4.42642
F37	-6.09058	-0.42936	-2.12767
F38	-4.38412	0.009301	-0.09212

F39	-0.90132	-2.02663	-2.59737
F40	-2.61945	-2.40701	-4.6518
O41	0.733355	0.866324	-1.97894
H42	0.996065	0.070175	-2.47486
H43	2.385942	1.469231	-0.0372
O44	3.076839	4.455416	-0.7917
O45	3.15613	1.867735	-1.91449
O46	2.580065	-0.60004	-3.72257
O47	4.357295	-0.54444	-1.54711
H48	3.769894	4.2918	-0.13963
H49	2.241202	4.353809	-0.26636
H50	3.16141	2.812614	-1.65073
H51	3.252654	-0.8025	-3.03763
H52	2.712886	0.351313	-3.83807
H53	4.0889	0.403442	-1.58147
O54	-1.23426	2.281099	-0.09583
H56	-0.59752	2.978668	0.178547
H57	-1.3708	2.411685	-1.06586
O58	-1.21938	2.357428	-2.82442
H59	-0.46284	1.716997	-2.6348
H60	-0.77013	3.179722	-3.05809
O61	0.921055	3.793541	0.697785
H62	1.291037	2.776379	0.737706
H63	0.840209	4.074747	1.617813
H64	2.1638	-1.08558	0.624674
C64	1.309568	-1.29756	-0.03042
H65	0.753017	-2.1517	0.37019
H66	1.646754	-1.53854	-1.04385

Table S76. $[Rh^{III}(NN^{F})(OH)_2(H_2O^{eq})(CH_3^{ax})]^{-}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.362222	-0.06188	-0.1092
N2	-0.78692	-0.22005	1.639982
H3	3.533464	0.068857	0.544346
C4	-1.86195	-0.70212	1.006813
O5	2.124062	0.853862	0.455092
N6	-1.59182	-0.89093	-0.27681
H7	2.102004	-0.20948	-2.09293
C8	-5.71724	-1.37591	2.797225
C9	-5.12084	-2.3726	2.030347

C10	-3.87046	-2.14831	1.463472
C11	-3.18911	-0.94006	1.639136
C12	-3.81456	0.044859	2.410467
C13	-5.06215	-0.16309	2.99068
F14	-6.91789	-1.58353	3.347827
F15	-5.7482	-3.54208	1.850984
F16	-3.32371	-3.13611	0.747009
F17	-3.22685	1.231975	2.600597
F18	-5.64118	0.797772	3.721392
C19	0.105696	-0.24964	5.759335
C20	-0.54762	-1.33643	5.189473
C21	-0.84871	-1.33351	3.832181
C22	-0.54479	-0.24225	2.997145
C23	0.133166	0.830491	3.604971
C24	0.455417	0.832691	4.956425
F25	0.400118	-0.24581	7.068142
F26	-0.86438	-2.3972	5.947994
F27	-1.42062	-2.43648	3.314845
F28	0.478013	1.898741	2.870226
F29	1.085877	1.883246	5.499224
C30	-4.20853	-1.06857	-3.56569
C31	-4.4202	-0.11782	-2.57313
C32	-3.57324	-0.06954	-1.47177
C33	-2.50978	-0.97275	-1.30988
C34	-2.31606	-1.9137	-2.33481
C35	-3.14948	-1.964	-3.4462
F36	-5.02264	-1.12594	-4.63019
F37	-5.43276	0.753561	-2.68849
F38	-3.78642	0.887088	-0.55229
F39	-1.31713	-2.79538	-2.24692
F40	-2.95154	-2.88556	-4.40059
O41	1.102915	-0.19634	-2.08173
H42	0.893232	0.629759	-2.58184
H43	1.852843	1.410145	1.197342
O44	2.732344	2.694397	-1.40134
O45	1.232158	2.116761	-3.4894
O46	3.772132	0.152839	-2.24115
O47	4.440853	-0.33021	0.365875
H48	2.483887	2.005311	-0.71864
H49	2.166239	3.467331	-1.11079

H50	1.81869	2.399137	-2.71923
H51	1.837909	1.900155	-4.20874
H52	4.119575	-0.14996	-1.36569
H53	3.714398	1.117892	-2.13016
H54	5.054474	0.38698	0.570456
O55	-0.50022	1.959267	-0.47354
H56	0.972441	-2.54925	-0.67344
H57	-1.2355	2.032861	0.148832
H58	-0.36748	3.216229	-3.19829
O59	-1.03067	3.578623	-2.58807
H60	-1.00171	2.903678	-1.85826
H61	0.360648	3.406987	-0.29246
O62	0.788703	4.279699	-0.54414
H63	0.24893	4.45879	-1.34117
C64	1.16502	-1.94084	0.21577
H65	2.242124	-1.8563	0.387886
H66	0.695276	-2.41952	1.084003

Table S77. $Rh^{III}(NN^{F})(OH^{ax})(H_2O)_2(CH_3^{ax})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.339297	0.117035	-0.11341
N2	-0.632	-0.46627	1.666694
H3	2.23199	1.199392	1.352379
C4	-1.6547	-0.99898	1.016426
O5	2.178087	1.048344	0.370367
N6	-1.46703	-0.89673	-0.29865
H7	0.009812	0.668019	-2.65766
C8	-5.06015	-2.88738	2.827305
C9	-4.28841	-3.58233	1.898363
C10	-3.18872	-2.95835	1.31868
C11	-2.83402	-1.64625	1.64823
C12	-3.62648	-0.97045	2.580939
C13	-4.73009	-1.57769	3.171776
F14	-6.11647	-3.47536	3.386124
F15	-4.60364	-4.83838	1.574136
F16	-2.46285	-3.64971	0.433413
F17	-3.33982	0.292142	2.917695
F18	-5.47738	-0.91271	4.055877
C19	0.252112	-1.06831	5.738134
C20	0.218848	-2.15576	4.86832

C21	-0.08556	-1.9511	3.527757
C22	-0.37056	-0.67543	3.021862
C23	-0.35063	0.394274	3.923478
C24	-0.03423	0.209197	5.264155
F25	0.546321	-1.25378	7.027867
F26	0.479776	-3.38621	5.324441
F27	-0.11748	-3.01028	2.702878
F28	-0.66807	1.620792	3.501129
F29	-0.02448	1.249257	6.104587
C30	-4.39097	-1.03142	-3.32495
C31	-4.56918	-0.19596	-2.22504
C32	-3.60922	-0.16965	-1.22126
C33	-2.46312	-0.97661	-1.26268
C34	-2.31517	-1.80061	-2.38438
C35	-3.25546	-1.83374	-3.40625
F36	-5.30494	-1.06542	-4.29764
F37	-5.65006	0.58551	-2.14895
F38	-3.77665	0.67706	-0.18913
F39	-1.23256	-2.6031	-2.4871
F40	-3.08261	-2.6413	-4.45804
O41	0.852313	0.480699	-2.16045
H42	1.224885	-0.33732	-2.58179
H43	2.226831	1.969073	-0.01938
O44	2.265822	3.648026	-0.33278
O45	-1.32757	1.36755	-3.47325
O46	1.48952	-1.83662	-3.3443
O47	2.129369	1.811779	2.935607
H48	1.660189	3.837009	-1.07244
H49	1.737298	3.903476	0.453907
H50	-1.02389	2.2497	-3.1377
H51	-1.21243	1.410463	-4.4314
H52	0.6161	-2.2468	-3.25202
H53	2.041199	-2.31059	-2.7063
H54	1.481595	2.51843	2.679777
H55	2.945894	2.275196	3.160131
O56	-0.62946	2.151983	-0.02641
H57	-1.58217	2.028226	0.074818
H58	1.489681	-2.04193	0.879389
O59	0.511083	3.571923	1.736039
O60	0.126416	3.26243	-2.22638

H61	-0.24018	2.895019	-1.34372
H62	0.821262	2.616934	-2.43235
H63	-0.09651	4.184361	2.166402
H64	-0.04706	2.983093	1.085594
C65	1.364407	-1.67256	-0.14112
H66	0.815754	-2.42075	-0.7204
H67	2.352477	-1.47288	-0.56949

Table S78. $Rh^{III}(NN^{F})(OH^{eq})(H_2O)_2(CH_3{}^{ax})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.432073	0.018364	-0.09835
N2	-0.77193	0.065922	1.628805
H3	3.545179	-0.05977	0.67233
C4	-1.83621	-0.46604	1.000513
O5	2.225602	0.942853	0.443246
N6	-1.53465	-0.71235	-0.26312
H7	2.239013	-0.43393	-2.01297
C8	-5.69915	-1.17876	2.768464
C9	-5.09109	-2.16034	1.990052
C10	-3.84078	-1.91949	1.429399
C11	-3.16832	-0.70585	1.618026
C12	-3.80705	0.255268	2.40605
C13	-5.05326	0.037099	2.980319
F14	-6.89405	-1.4015	3.31109
F15	-5.7032	-3.32912	1.794971
F16	-3.28217	-2.89579	0.710706
F17	-3.22365	1.450573	2.635825
F18	-5.63208	0.983571	3.722608
C19	0.205011	-0.10578	5.734548
C20	-0.46445	-1.1718	5.14115
C21	-0.79616	-1.12429	3.791315
C22	-0.50738	-0.0075	2.985919
C23	0.187753	1.034421	3.619194
C24	0.543272	1.001518	4.960399
F25	0.527182	-0.14668	7.029686
F26	-0.7673	-2.25245	5.865623
F27	-1.37579	-2.20793	3.248647
F28	0.543365	2.129256	2.89732
F29	1.193654	2.030892	5.511483
C30	-4.09103	-1.06683	-3.58226

C31	-4.29359	-0.04103	-2.66412
C32	-3.46784	0.054928	-1.55179
C33	-2.43498	-0.86234	-1.31289
C34	-2.24729	-1.88015	-2.2586
C35	-3.0631	-1.98481	-3.37994
F36	-4.88018	-1.17037	-4.65574
F37	-5.26691	0.85594	-2.86337
F38	-3.65321	1.084209	-0.70194
F39	-1.27205	-2.77391	-2.08521
F40	-2.87488	-2.97183	-4.26175
O41	1.232146	-0.34677	-2.02364
H42	1.065334	0.425897	-2.60696
H43	1.985451	1.470801	1.216629
O44	2.979032	2.360481	-1.57248
O45	1.195019	1.996688	-3.50863
O46	3.860966	-0.26461	-2.08281
O47	4.319	-0.68015	0.567712
H48	2.623275	1.882018	-0.73828
H49	3.283672	3.230519	-1.2891
H50	1.797951	2.308061	-2.77652
H51	1.763493	1.832344	-4.27129
H52	4.165327	-0.55864	-1.18968
H53	3.897645	0.707773	-2.02637
H54	5.086273	-0.21626	0.923834
O55	-0.23982	2.158618	-0.78085
H56	0.450339	-2.26674	1.215827
H57	-0.59103	2.200146	-3.52217
O58	-1.51727	2.215374	-3.19935
H59	-0.8431	2.148217	-1.5569
H60	-0.7192	2.641663	-0.07208
O61	-1.54511	3.43008	1.267568
H62	-0.92557	3.192651	1.972039
H63	-2.31602	2.872552	1.438915
H64	-1.82576	3.116698	-3.3557
C65	1.076564	-1.85301	0.420342
H66	0.984937	-2.47191	-0.4753
H67	2.117122	-1.79162	0.745648

Table S79. $Rh^{III}(NN^{F})(OH^{ax})(H_2O)_2(CH_3^{eq})\cdot 6H_2O$

Atom	x	y	z

Rh1	0.383374	0.261643	-0.23472
N2	-0.8445	-0.08753	1.953984
H3	3.077859	0.565433	0.191032
C4	-1.71876	-0.71848	1.178725
O5	2.277981	1.221602	0.053495
N6	-1.4795	-0.62366	-0.12972
H7	0.004823	0.817173	-2.7264
C8	-5.14666	-2.84035	2.701156
C9	-4.24163	-3.49335	1.866732
C10	-3.13964	-2.80116	1.375548
C11	-2.91017	-1.46052	1.698824
C12	-3.83494	-0.83334	2.537257
C13	-4.9452	-1.50367	3.038979
F14	-6.20546	-3.49362	3.175184
F15	-4.43251	-4.77559	1.550281
F16	-2.28271	-3.45717	0.583994
F17	-3.675	0.458892	2.87208
F18	-5.81628	-0.87533	3.831326
C19	0.185015	-1.08527	5.924517
C20	-0.03785	-2.0985	4.9965
C21	-0.41301	-1.78417	3.696037
C22	-0.59779	-0.45834	3.265888
C23	-0.33972	0.52912	4.227305
C24	0.039767	0.242526	5.530575
F25	0.540257	-1.38165	7.178326
F26	0.127731	-3.37611	5.355133
F27	-0.56008	-2.79377	2.819032
F28	-0.46007	1.837801	3.866506
F29	0.257908	1.230062	6.406358
C30	-4.27996	-1.3073	-3.2077
C31	-4.54949	-0.3591	-2.22401
C32	-3.6304	-0.1546	-1.20167
C33	-2.43639	-0.88244	-1.11485
C34	-2.20098	-1.83772	-2.11193
C35	-3.10145	-2.04872	-3.15064
F36	-5.15209	-1.51141	-4.19685
F37	-5.67951	0.352973	-2.27164
F38	-3.91537	0.773159	-0.26399
F39	-1.08875	-2.58477	-2.06453
F40	-2.85126	-2.97046	-4.08391

H41	0.631704	-0.86448	-2.56023
H42	2.174733	1.677684	0.917118
O43	1.769389	2.848303	2.244173
O44	4.191814	-0.35594	0.520752
H45	1.63508	3.96735	0.476028
H46	2.449078	2.947085	2.923591
H47	4.137421	-0.9898	-0.23893
H48	3.798906	-0.86153	1.272954
O49	-0.50206	2.175834	-0.59702
O50	1.213604	-1.58262	0.034758
H51	-1.82459	1.904436	2.000728
H52	0.497892	-2.21118	-0.13492
O53	2.587943	-1.72107	2.28293
O54	3.399199	-2.02148	-1.44013
H55	2.888572	-2.62954	2.411201
H56	1.967669	-1.75775	1.500255
H57	2.516501	-1.93205	-0.98876
H58	3.296734	-1.55442	-2.27851
O59	-2.16143	2.631529	1.451075
O60	1.573431	3.87384	-0.48942
H61	-1.13332	2.416714	0.128654
H62	-3.02754	2.320555	1.154798
H63	2.165685	3.120891	-0.66541
H64	0.192421	2.887927	-0.6278
C65	0.735633	0.171871	-2.23272
H66	1.750304	0.539359	-2.41553
H67	0.96357	2.583293	2.715749

Table S80. $Rh^{III}(NN^{F})(OH^{eq})(H_2O)_2(CH_3{}^{eq})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.420047	0.174738	-0.4065
N2	-0.56356	-0.34145	1.692312
H3	3.545818	0.238666	0.342251
C4	-1.57264	-0.8688	1.012114
O5	2.220761	1.190467	-0.08212
N6	-1.42176	-0.7952	-0.30939
H7	-0.91431	4.244357	-2.49491
C8	-5.02839	-2.638	2.873107
C9	-4.28707	-3.36977	1.948015
C10	-3.17447	-2.78913	1.347296

C11	-2.77624	-1.48383	1.648939
C12	-3.53785	-0.77239	2.580418
C13	-4.65409	-1.33439	3.191685
F14	-6.09604	-3.18573	3.454411
F15	-4.64252	-4.62298	1.649618
F16	-2.47671	-3.52101	0.472635
F17	-3.20957	0.484364	2.901798
F18	-5.36945	-0.63082	4.074486
C19	0.355925	-1.05436	5.750299
C20	0.06437	-2.12534	4.909217
C21	-0.26037	-1.89231	3.575994
C22	-0.32804	-0.5946	3.031443
C23	-0.01648	0.456154	3.910603
C24	0.320308	0.242148	5.241828
F25	0.670964	-1.26771	7.032081
F26	0.112772	-3.3756	5.381695
F27	-0.49343	-2.95277	2.784614
F28	-0.05959	1.7299	3.46752
F29	0.597894	1.277851	6.041933
C30	-4.40453	-1.16935	-3.2637
C31	-4.61756	-0.33661	-2.16881
C32	-3.63978	-0.22393	-1.18605
C33	-2.43759	-0.94729	-1.24523
C34	-2.25261	-1.77554	-2.36319
C35	-3.21393	-1.8854	-3.362
F36	-5.33503	-1.27905	-4.2172
F37	-5.75162	0.368536	-2.07662
F38	-3.86015	0.61811	-0.16512
F39	-1.124	-2.48537	-2.48735
F40	-3.00656	-2.68815	-4.41268
H41	0.500449	-0.68	-2.85853
H42	2.474693	1.603291	-0.92011
O43	1.173158	5.25701	-0.43328
O44	-0.11178	3.765208	-2.25322
O45	3.525557	-1.65628	-2.13151
O46	4.271723	-0.41757	0.532348
H47	2.084554	5.518388	-0.60975
H48	1.221152	4.627758	0.322818
H49	0.4015	4.390795	-1.67725
H50	3.698932	-2.52571	-2.51634

H51	3.213187	-1.10283	-2.86084
H52	4.415575	-0.84706	-0.32432
O53	-0.61677	1.997928	-0.34262
O54	1.334268	-1.70766	-0.4102
H55	-0.15833	2.494983	0.380639
H56	-0.47625	2.56931	-1.15145
O57	1.217916	3.144648	1.258182
H58	1.743618	2.38605	0.827164
H59	1.08058	2.9141	2.186088
H60	1.733975	-1.91442	0.492488
H61	2.093575	-1.70914	-1.02908
O62	2.699271	-2.15112	1.763789
H63	2.351424	-1.76291	2.575562
H64	3.411834	-1.52821	1.442838
C65	0.702758	0.304066	-2.427
H66	0.025601	1.047967	-2.85526
H67	1.733997	0.613085	-2.65475

Table S81. $[Rh^{IV}(NN^{F})(OH)_3(CH_3^{ax})]^{-}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.277824	0.235767	-0.14784
N2	-0.80839	-0.29818	1.63919
H3	3.259449	0.721564	-0.39751
C4	-1.7955	-0.89047	0.983829
O5	1.819976	1.072116	0.684525
N6	-1.62711	-0.78459	-0.33041
H7	1.807584	1.910012	-2.34044
C8	-5.14355	-2.80541	2.892618
C9	-4.43429	-3.47643	1.900589
C10	-3.35214	-2.85293	1.286416
C11	-2.95273	-1.5612	1.641264
C12	-3.68458	-0.90993	2.639577
C13	-4.76926	-1.51736	3.264091
F14	-6.18558	-3.39642	3.486434
F15	-4.79311	-4.71756	1.54933
F16	-2.69259	-3.53088	0.343723
F17	-3.36724	0.3342	3.013384
F18	-5.45969	-0.86827	4.210445
C19	0.741427	-1.07393	5.470129
C20	0.290979	-2.13308	4.690016

C21	-0.24222	-1.88995	3.429025
C22	-0.36692	-0.5872	2.917763
C23	0.104611	0.460761	3.726928
C24	0.651755	0.226794	4.98238
F25	1.251172	-1.30284	6.688894
F26	0.379792	-3.38827	5.154908
F27	-0.64168	-2.94307	2.702474
F28	0.01507	1.722859	3.296702
F29	1.075522	1.249361	5.738941
C30	-4.49556	-1.09066	-3.40034
C31	-4.81035	-0.40743	-2.23069
C32	-3.86959	-0.31087	-1.21199
C33	-2.59958	-0.90803	-1.30199
C34	-2.3088	-1.5735	-2.50607
C35	-3.23573	-1.66691	-3.53764
F36	-5.39673	-1.19133	-4.38834
F37	-6.01318	0.172519	-2.09833
F38	-4.19331	0.40852	-0.12174
F39	-1.11416	-2.14817	-2.68116
F40	-2.92953	-2.32742	-4.66323
O41	0.737323	0.422491	-2.01216
H42	1.419542	-0.25799	-2.23137
H43	1.795334	2.058422	0.601267
O44	1.975195	3.737801	0.035072
O45	2.559786	2.542116	-2.32065
O46	2.846691	-1.23102	-2.72804
O47	4.036732	0.550051	-0.97313
H48	1.047382	3.985403	-0.06394
H49	2.232241	3.421611	-0.87241
H50	3.288834	1.971328	-1.99439
H51	2.423521	-2.12095	-2.42841
H52	2.988812	-1.27555	-3.67982
H53	3.7306	-0.16511	-1.57251
O55	1.227889	-1.70559	0.099478
H56	-0.57276	2.624036	0.626359
H57	-0.38336	2.585276	-1.17154
H64	2.053109	-1.5773	0.597776
O65	3.673533	-0.814	1.654559
H66	3.027768	-0.08371	1.646375
H67	4.188504	-0.61341	0.855863

O68	1.635924	-3.24992	-1.78987
H69	0.76545	-3.28073	-2.20719
H70	1.453518	-2.63492	-0.92097
C64	-0.74313	2.049453	-0.28896
H65	-1.81565	1.859429	-0.39023

Table S82. $Rh^{IV}(NN^{F})(OH)_2(H_2O^{ax})(CH_3^{ax})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.308054	-0.00627	-0.2332
N2	-0.70255	-0.39282	1.618556
H3	3.419028	0.637503	-0.56485
C4	-1.76372	-0.95825	1.033156
O5	1.864472	0.907171	0.486713
N6	-1.59536	-0.99002	-0.27996
H7	1.666701	1.596136	-2.366
C8	-5.19413	-2.45958	3.142386
C9	-4.59258	-3.23094	2.150426
C10	-3.4841	-2.73466	1.47203
C11	-2.95337	-1.4716	1.757947
C12	-3.57773	-0.71932	2.758432
C13	-4.68544	-1.19875	3.448509
F14	-6.25416	-2.92663	3.798523
F15	-5.07374	-4.44204	1.863029
F16	-2.92099	-3.50853	0.539917
F17	-3.12365	0.502677	3.070582
F18	-5.2661	-0.45641	4.395005
C19	0.803432	-1.04766	5.50213
C20	0.275968	-2.11402	4.779218
C21	-0.23447	-1.90101	3.503756
C22	-0.26293	-0.62602	2.911444
C23	0.288828	0.419171	3.666297
C24	0.815356	0.224605	4.936007
F25	1.296866	-1.24212	6.726704
F26	0.278101	-3.34206	5.304613
F27	-0.68649	-2.96276	2.816691
F28	0.32805	1.671676	3.160623
F29	1.320066	1.255658	5.620854
C30	-4.43097	-1.0462	-3.38273
C31	-4.69098	-0.30259	-2.23494
C32	-3.77072	-0.29471	-1.19358

C33	-2.58343	-1.04124	-1.2534
C34	-2.34421	-1.77596	-2.42585
C35	-3.25088	-1.78046	-3.4794
F36	-5.31079	-1.05701	-4.38668
F37	-5.81812	0.411993	-2.14247
F38	-4.03506	0.462754	-0.11744
F39	-1.22387	-2.49184	-2.539
F40	-3.00279	-2.496	-4.58044
O41	0.704635	0.06906	-2.13724
H42	1.406362	-0.5793	-2.40897
H43	1.763988	1.870879	0.341548
O44	1.784921	3.721082	0.006118
O45	2.124333	2.448437	-2.5468
O46	2.934691	-1.32471	-2.76552
O47	4.023038	0.678487	-1.33619
H48	2.554392	4.106851	0.442072
H49	0.999474	3.983726	0.525219
H50	1.962812	2.986692	-1.75081
H51	3.479817	-0.66342	-2.2612
H52	3.218525	-1.25509	-3.68497
H53	3.654946	1.420946	-1.85361
O54	-1.04618	1.889068	-0.6313
H56	-0.95425	2.66076	-0.04949
H57	-0.95289	2.180676	-1.57601
O58	-0.64643	2.228549	-3.26173
H59	-0.37148	1.292254	-3.19896
H60	0.217293	2.672842	-3.3396
O61	-0.55886	3.768163	1.438869
H62	-0.4951	3.062676	2.101755
H63	-1.24729	4.374554	1.738154
H64	2.091749	-1.53066	0.830702
C64	1.334414	-1.75721	0.078068
H65	0.627515	-2.50785	0.435172
H66	1.793857	-2.0663	-0.86047

Table S83. $Rh^{IV}(NN^{F})(OH)_2(H_2O^{eq})(CH_3^{ax})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.345986	0.005651	-0.09767
N2	-0.77473	-0.21905	1.626936
H3	3.503791	-0.12736	0.546528

C4	-1.84473	-0.7298	1.007596
O5	2.048334	0.829351	0.532254
N6	-1.56833	-0.90886	-0.27922
H7	2.151388	-0.07622	-2.07466
C8	-5.66113	-1.51437	2.806079
C9	-5.03761	-2.49809	2.040377
C10	-3.79783	-2.23709	1.467193
C11	-3.15577	-1.00682	1.642975
C12	-3.80532	-0.03554	2.412398
C13	-5.04485	-0.27825	2.994697
F14	-6.84764	-1.75528	3.357278
F15	-5.62698	-3.68168	1.865463
F16	-3.21733	-3.20054	0.745616
F17	-3.24417	1.166929	2.589329
F18	-5.6487	0.664919	3.719012
C19	0.084888	-0.08944	5.749568
C20	-0.51083	-1.22368	5.204347
C21	-0.78897	-1.27438	3.842762
C22	-0.52351	-0.18936	2.991326
C23	0.1004	0.925993	3.568277
C24	0.404793	0.985579	4.922633
F25	0.359988	-0.037	7.053272
F26	-0.7926	-2.26979	5.984549
F27	-1.30337	-2.40745	3.338267
F28	0.433302	1.971262	2.78669
F29	0.991029	2.06896	5.435124
C30	-4.26001	-1.10246	-3.50739
C31	-4.41877	-0.11584	-2.53684
C32	-3.53626	-0.06448	-1.46532
C33	-2.49804	-0.99574	-1.31188
C34	-2.3545	-1.96794	-2.31112
C35	-3.22271	-2.0258	-3.39642
F36	-5.09997	-1.16236	-4.54119
F37	-5.40536	0.777076	-2.64515
F38	-3.68672	0.917731	-0.55549
F39	-1.37171	-2.86835	-2.22615
F40	-3.07435	-2.97081	-4.3276
O41	1.141553	-0.06434	-2.04786
H42	0.926616	0.754674	-2.56463
H43	1.838167	1.28153	1.363715

O44	2.806543	2.775041	-1.32579
O45	1.318879	2.211567	-3.45542
O46	3.759059	0.182556	-2.22518
O47	4.259565	-0.70272	0.280923
H48	2.577222	2.077012	-0.67259
H49	2.217881	3.523387	-1.03027
H50	1.937882	2.492362	-2.71955
H51	1.871408	2.034619	-4.22729
H52	4.134008	-0.21429	-1.40303
H53	3.858057	1.140884	-2.1025
H54	5.025269	-0.4015	0.784557
O55	-0.66344	1.731736	-0.68563
H56	0.74814	-2.43569	-0.94811
H57	-1.5014	1.784627	-0.20144
H58	-0.16374	3.421223	-3.27228
O59	-0.86175	3.7576	-2.68255
H60	-1.02253	2.973278	-2.12293
H61	0.325024	3.420593	-0.19504
O62	0.743765	4.248671	-0.49644
H63	0.218545	4.408593	-1.31418
C64	0.987233	-1.98177	0.010237
H65	2.063688	-1.90761	0.177083
H66	0.472107	-2.47505	0.834593

Table S84. $Rh^{IV}(NN^{F})(OH)_2(H_2O^{ax})(CH_3^{eq})\cdot 6H_2O$

Atom	x	y	z
Rh1	0.363052	0.219554	-0.13535
N2	-0.80693	-0.31447	1.878857
H3	2.634108	0.874313	0.766556
C5	-1.74106	-0.89213	1.129713
O6	1.851776	1.364872	0.336181
N7	-1.48141	-0.81764	-0.17379
H7	-0.02046	0.734057	-2.63978
C20	-5.34449	-2.60921	2.729123
C21	-4.58287	-3.33126	1.812016
C22	-3.41788	-2.7725	1.298014
C23	-2.98404	-1.49933	1.680645
C24	-3.76707	-0.79806	2.604571
C25	-4.93735	-1.33741	3.12767
F26	-6.46104	-3.1357	3.226197

F27	-4.96872	-4.55309	1.439622
F28	-2.70063	-3.494	0.42993
F29	-3.40875	0.429142	3.008011
F30	-5.66984	-0.64469	4.001412
C31	0.369789	-1.50113	5.743129
C32	-0.0196	-2.46586	4.818704
C33	-0.43539	-2.07915	3.553351
C34	-0.49875	-0.7283	3.16381
C35	-0.08038	0.213997	4.118038
C36	0.344302	-0.15423	5.38647
F37	0.76785	-1.86321	6.963675
F38	0.030395	-3.76092	5.145404
F39	-0.73982	-3.0402	2.664468
F40	-0.09414	1.521009	3.801254
F41	0.715922	0.774892	6.272157
C42	-4.31456	-0.99718	-3.2824
C43	-4.50368	-0.10628	-2.22802
C44	-3.57835	-0.06313	-1.19119
C45	-2.45586	-0.9029	-1.1714
C46	-2.2925	-1.78848	-2.24395
C47	-3.20475	-1.84014	-3.29167
F48	-5.1973	-1.04699	-4.28097
F49	-5.5643	0.705269	-2.22231
F50	-3.76831	0.807054	-0.19036
F51	-1.23738	-2.61662	-2.26424
F52	-3.03103	-2.69993	-4.29885
H42	0.513814	-0.98322	-2.42406
H43	1.412826	2.695093	1.425451
O44	1.069729	3.541463	1.803471
O47	3.91974	0.203166	1.39783
H45	1.213948	4.196818	-0.21806
H46	1.574233	3.704175	2.609806
H47	4.196656	-0.34813	0.63012
H48	3.545254	-0.46317	2.016845
O56	-0.75427	1.971429	-0.57516
O57	1.425215	-1.49579	0.147249
H51	-0.69473	3.254839	1.937097
H52	0.846478	-2.21002	-0.15643
O60	2.523044	-1.8709	2.570148
O61	3.97621	-1.50184	-0.74608

H55	3.094975	-2.64532	2.49197
H56	2.037326	-1.82134	1.7059
H57	3.005726	-1.56385	-0.5643
H58	4.052094	-1.0576	-1.5991
O66	-1.59279	2.924468	1.705983
O67	1.250625	3.677193	-1.03899
H61	-1.1917	2.31808	0.264177
H62	-1.72392	2.159877	2.282676
H63	1.820961	2.928655	-0.77317
H64	-0.10554	2.680452	-0.85312
C65	0.679467	0.05768	-2.14912
H66	1.71693	0.349634	-2.3194

Table S85. $[Rh^{II}(NN^{F})(OH)_2]^{-}\cdot 4H_2O$

Atom	x	y	z
Rh1	0.413147	0.238661	-0.33389
N2	-0.5447	-0.32757	1.534178
H3	3.458088	0.55089	-0.34462
C4	-1.6056	-0.85101	0.924435
O5	1.984054	1.23241	0.369202
N6	-1.49713	-0.74949	-0.39683
H7	1.817213	1.629273	-2.51707
C8	-4.96266	-2.63454	2.946499
C9	-4.29613	-3.33861	1.947728
C10	-3.21082	-2.75401	1.302833
C11	-2.76658	-1.4687	1.627292
C12	-3.45517	-0.7854	2.634233
C13	-4.54135	-1.35376	3.292754
F14	-6.00674	-3.18817	3.572869
F15	-4.69598	-4.57516	1.622952
F16	-2.58613	-3.4674	0.359891
F17	-3.0891	0.452346	2.984855
F18	-5.18992	-0.67467	4.248195
C19	0.792162	-1.02382	5.468065
C20	0.364511	-2.09313	4.688974
C21	-0.09421	-1.86564	3.396692
C22	-0.16548	-0.57634	2.840736
C23	0.287011	0.480785	3.650303
C24	0.758859	0.264142	4.940476
F25	1.231044	-1.23143	6.719426

F26	0.410814	-3.34141	5.182426
F27	-0.44952	-2.93286	2.656568
F28	0.251168	1.732286	3.189259
F29	1.164577	1.295989	5.69535
C30	-4.50865	-1.01386	-3.32747
C31	-4.74034	-0.2765	-2.17151
C32	-3.75767	-0.20338	-1.1909
C33	-2.52707	-0.87054	-1.31287
C34	-2.32069	-1.60065	-2.49694
C35	-3.29197	-1.67106	-3.4897
F36	-5.45315	-1.09526	-4.27769
F37	-5.90555	0.372735	-2.01424
F38	-3.99938	0.560469	-0.10903
F39	-1.17941	-2.26613	-2.67671
F40	-3.07489	-2.39157	-4.59977
O41	0.761238	0.286705	-2.26401
H42	1.397816	-0.44752	-2.40691
H43	1.70924	2.168271	0.349507
O44	0.568031	3.643329	-0.66208
O45	2.479167	2.360861	-2.37999
O46	2.608956	-1.88079	-1.94128
O47	4.128756	0.198724	-0.98084
H48	-0.07678	2.919495	-0.63172
H49	1.095747	3.431546	-1.45687
H50	2.652435	2.248244	-1.43192
H51	3.250377	-1.23348	-1.55997
H52	2.000073	-2.05081	-1.20868
H53	3.97598	0.75755	-1.75947

Table S86. $Rh^{II}(NN^{F})(OH)(H_2O)\cdot 4H_2O$

Atom	x	y	z
Rh1	0.403198	-0.13247	-0.06616
N2	-0.79832	-0.11017	1.650811
H3	3.454862	0.242351	0.537927
C4	-1.84582	-0.62925	1.009997
O5	1.943482	1.100109	0.418661
N6	-1.50242	-0.88976	-0.25936
H7	2.170602	-0.30197	-2.07251
C8	-5.75869	-1.2596	2.666211
C9	-5.12725	-2.28465	1.964268

C10	-3.85798	-2.07405	1.436329
C11	-3.19382	-0.85191	1.588047
C12	-3.85451	0.16133	2.291346
C13	-5.12075	-0.03241	2.832791
F14	-6.97269	-1.45287	3.177373
F15	-5.73702	-3.46185	1.811484
F16	-3.26992	-3.08262	0.785297
F17	-3.28057	1.359676	2.446999
F18	-5.72857	0.951974	3.498748
C19	-0.12312	0.161139	5.806162
C20	-0.73816	-0.97192	5.281475
C21	-0.96807	-1.06804	3.91298
C22	-0.62784	-0.03199	3.02574
C23	0.010486	1.083853	3.587588
C24	0.263358	1.189233	4.949405
F25	0.103901	0.257844	7.117861
F26	-1.08742	-1.97553	6.091249
F27	-1.50364	-2.20486	3.442001
F28	0.405173	2.09417	2.787206
F29	0.866058	2.275888	5.440961
C30	-4.00891	-1.43705	-3.59511
C31	-4.26573	-0.39534	-2.70754
C32	-3.45183	-0.22509	-1.59407
C33	-2.38218	-1.09096	-1.32158
C34	-2.14	-2.12594	-2.23682
C35	-2.94027	-2.29963	-3.36154
F36	-4.78492	-1.608	-4.6682
F37	-5.28106	0.444371	-2.93624
F38	-3.68986	0.815009	-0.77831
F39	-1.12679	-2.96831	-2.03119
F40	-2.69713	-3.29891	-4.21456
O41	1.168337	-0.406	-2.00187
H42	0.8103	0.32813	-2.57132
H43	1.730976	1.492522	1.277487
O44	2.508066	2.637435	-1.62581
O45	0.519577	1.828139	-3.30217
O46	3.722393	0.156478	-2.23993
O47	4.309158	-0.23034	0.386501
H48	2.266798	2.146601	-0.78131
H49	2.736519	3.540835	-1.37646

H50	1.181971	2.310738	-2.75442
H51	0.874878	1.838274	-4.19992
H52	4.114604	-0.08761	-1.36795
H53	3.601424	1.121821	-2.18023
H54	4.995545	0.348769	0.739068

Table S87. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_3{}^{ax}\text{-}H\text{-}OH^{eq})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.129316	0.615568	-0.12345
N2	-1.03567	0.468529	1.614779
H3	3.985252	-0.50583	0.244462
C4	-2.11837	0.061033	0.949739
O5	1.878482	1.653071	0.481236
N6	-1.82792	-0.05855	-0.34262
H7	1.604718	-0.04464	-2.24823
C8	-5.9999	-0.61366	2.655771
C9	-5.42225	-1.58451	1.839366
C10	-4.16096	-1.3617	1.297534
C11	-3.45279	-0.1823	1.550954
C12	-4.05498	0.774999	2.375714
C13	-5.31591	0.570105	2.926213
F14	-7.20675	-0.8175	3.178108
F15	-6.07538	-2.72044	1.588629
F16	-3.62478	-2.31442	0.527153
F17	-3.42901	1.926395	2.64229
F18	-5.87422	1.501151	3.70185
C19	-0.22588	0.028511	5.721836
C20	-0.78606	-1.03031	5.01117
C21	-1.05628	-0.88014	3.656368
C22	-0.81126	0.323349	2.976573
C23	-0.22847	1.363215	3.714843
C24	0.062483	1.224385	5.067558
F25	0.042743	-0.10517	7.022093
F26	-1.04048	-2.18912	5.626004
F27	-1.53929	-1.93585	2.975057
F28	0.065115	2.520625	3.109286
F29	0.607515	2.237207	5.746484
C30	-4.42488	-0.13888	-3.65157
C31	-4.57816	0.846437	-2.67915
C32	-3.72885	0.860696	-1.57922

C33	-2.72616	-0.10386	-1.4037
C34	-2.59291	-1.07891	-2.40119
C35	-3.42615	-1.10072	-3.51391
F36	-5.23391	-0.16268	-4.71187
F37	-5.527	1.77751	-2.81329
F38	-3.86423	1.84266	-0.67083
F39	-1.65926	-2.03003	-2.27912
F40	-3.2859	-2.04953	-4.4429
O41	0.791282	0.595403	-2.08362
H42	1.121308	1.482291	-2.38841
H43	2.119284	1.203666	1.315381
O44	3.90429	2.331821	-1.0659
O45	2.019697	2.809079	-2.97709
O46	2.750358	-0.89147	-2.59732
O47	4.500421	-0.43156	-0.58429
H48	3.160196	2.100242	-0.44288
H49	4.366045	3.079704	-0.66625
H50	2.815692	2.731348	-2.40082
H51	2.315383	2.537785	-3.85572
H52	2.35494	-1.79088	-2.49164
H53	3.43619	-0.81071	-1.88448
H54	4.570513	0.525944	-0.74681
O55	0.776514	-1.34225	0.170534
H56	0.07248	-1.7904	0.661359
H57	3.022969	-1.19233	2.378728
O58	2.761538	-0.57615	1.684349
H59	2.024094	-1.0131	1.153032
H60	0.441485	-2.89926	-2.47916
O61	1.226009	-3.00608	-1.92637
H62	1.033842	-2.44454	-1.13329
H63	-0.36753	3.526559	0.634145
H64	-1.37268	2.601801	-0.44155
H65	0.812534	2.326858	0.322651
C66	-0.33328	2.861282	-0.23817
H67	0.082869	3.37159	-1.1098

Table S88. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_3{}^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.168275	0.519206	0.11622
N2	-0.99443	0.056806	1.806515

H3	4.042398	1.047037	-1.40587
C4	-2.02497	-0.38912	1.099828
O5	1.778807	1.512827	0.98903
N6	-1.77423	-0.29419	-0.20782
H7	1.114903	2.318238	-2.30617
C8	-5.6962	-1.86872	2.770873
C9	-5.02177	-2.61348	1.805314
C10	-3.83468	-2.12663	1.268314
C11	-3.29512	-0.90165	1.676245
C12	-3.994	-0.17315	2.645131
C13	-5.18272	-0.64434	3.19321
F14	-6.83388	-2.32731	3.289397
F15	-5.51306	-3.78911	1.406531
F16	-3.20611	-2.86912	0.350813
F17	-3.53443	1.011886	3.062039
F18	-5.83467	0.072173	4.111727
C19	-0.00291	-0.70305	5.825468
C20	-0.4633	-1.74383	5.024022
C21	-0.80391	-1.49621	3.698851
C22	-0.72164	-0.2097	3.142872
C23	-0.24694	0.817104	3.972725
C24	0.111594	0.579619	5.294545
F25	0.326831	-0.93303	7.098873
F26	-0.56335	-2.97942	5.525647
F27	-1.20863	-2.52687	2.94136
F28	-0.14082	2.061256	3.494068
F29	0.550236	1.580088	6.064828
C30	-4.64948	-0.12248	-3.28838
C31	-4.76147	0.720872	-2.18561
C32	-3.817	0.650077	-1.16813
C33	-2.74904	-0.26133	-1.19848
C34	-2.66987	-1.09606	-2.32145
C35	-3.59639	-1.03151	-3.35592
F36	-5.54727	-0.06198	-4.27426
F37	-5.76384	1.601781	-2.11734
F38	-3.92697	1.496484	-0.12955
F39	-1.68918	-2.01206	-2.40386
F40	-3.49086	-1.85187	-4.40627
O41	1.005466	0.775885	-1.75359
H42	1.963609	0.615081	-1.59316

H43	2.379694	1.882834	0.303681
O44	3.510522	2.790635	-0.94965
O45	1.407336	3.263017	-2.48626
O46	3.697443	-1.42358	-3.56803
O47	3.736486	0.122411	-1.36733
H48	3.938795	3.566716	-0.57052
H49	2.808634	3.117285	-1.57765
H50	1.514154	3.335062	-3.44255
H51	2.748191	-1.61972	-3.39564
H52	4.158573	-2.25197	-3.38599
H53	3.914955	-0.34584	-2.21852
O54	0.881941	-1.49533	0.112739
H55	-1.49227	2.328757	0.027543
H56	-0.57957	3.261031	1.177067
H57	0.644917	2.210217	0.715555
H58	1.810479	-1.41757	0.514001
H59	0.989651	-1.75808	-0.8314
O60	3.201346	-0.89498	1.108407
H61	2.835812	-0.03962	1.414238
H62	3.62544	-0.63663	0.259774
O63	1.119387	-1.64389	-2.64993
H64	0.942634	-0.66397	-2.46601
H65	0.3069	-1.99478	-3.03609
C66	-0.4889	2.697161	0.240992
H67	-0.14487	3.318322	-0.58688

Table S89. $[Rh^{III}(NN^{F})(OH)_2(CH_3{}^{ax}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	-0.10578	0.687257	-0.12945
N2	-0.99698	0.308175	1.795384
H3	5.053096	-0.01036	0.896024
C4	-2.17947	0.043249	1.25248
O5	1.833312	1.378081	0.314564
N6	-2.15691	0.245625	-0.06166
H7	1.36029	1.867612	-2.52287
C8	-5.6021	-1.3	3.49193
C9	-5.17354	-2.01954	2.380471
C10	-4.06842	-1.57802	1.658223
C11	-3.37195	-0.42088	2.019095
C12	-3.82608	0.282853	3.138472

C13	-4.92751	-0.14394	3.873505
F14	-6.6626	-1.7181	4.191743
F15	-5.82033	-3.13558	2.019571
F16	-3.67993	-2.30167	0.605412
F17	-3.21235	1.406035	3.528008
F18	-5.34832	0.553608	4.936957
C19	0.56633	-0.96928	5.488509
C20	-0.13569	-1.86907	4.695198
C21	-0.67522	-1.45143	3.484437
C22	-0.55183	-0.12715	3.03291
C23	0.169546	0.754304	3.854563
C24	0.723059	0.345519	5.06145
F25	1.084102	-1.36387	6.661963
F26	-0.28026	-3.14159	5.097882
F27	-1.31486	-2.36185	2.733197
F28	0.331197	2.028151	3.478289
F29	1.393205	1.217053	5.83069
C30	-5.36812	0.65688	-2.7534
C31	-5.41735	1.296913	-1.52047
C32	-4.36121	1.157458	-0.62734
C33	-3.23848	0.359741	-0.91102
C34	-3.21281	-0.26337	-2.17244
C35	-4.25706	-0.11598	-3.0793
F36	-6.38378	0.782974	-3.6219
F37	-6.47451	2.06296	-1.20513
F38	-4.42485	1.837725	0.532607
F39	-2.18256	-1.03553	-2.51324
F40	-4.21428	-0.73935	-4.26642
O41	0.221925	0.998367	-2.11804
H42	0.442988	0.118457	-2.47502
H43	2.361263	1.089143	-0.46705
O44	2.820309	4.160781	-0.69187
O45	2.217961	2.390812	-2.80756
O46	3.434022	0.236138	-1.72078
O47	4.874444	-0.79118	0.357041
H48	2.625406	3.665873	-1.51347
H49	2.789759	3.459802	-0.02614
H50	2.072782	2.670065	-3.71865
H51	2.804967	-0.46951	-2.0314
H52	3.260845	1.010828	-2.29863

H53	4.47619	-0.41587	-0.46162
O54	0.282497	-1.34928	-0.26445
H55	-0.70916	3.157697	1.029307
H56	0.454245	3.729472	-0.20005
H57	0.917966	2.240324	0.109587
H58	0.954423	-1.4635	0.438457
O59	2.384646	-0.9912	1.735555
H60	2.193494	-0.07603	1.450923
H61	3.230779	-1.17209	1.278485
O62	1.50633	-1.46793	-2.41589
H63	1.540168	-2.36079	-2.77548
H64	0.986714	-1.51182	-1.48606
C65	-0.28686	2.950968	0.045021
H66	-1.03986	2.999142	-0.74183

Table S90. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_3{}^{eq}\text{-}H\text{-}OH^{ax})]^{\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.216857	0.249324	-0.16135
N2	-1.01039	0.236839	1.617365
H3	4.234621	0.963331	-1.46036
C4	-1.96646	-0.42885	0.980381
O5	1.969451	1.232801	0.57104
N6	-1.63762	-0.63539	-0.29346
H7	1.683435	-0.85892	-2.6716
C8	-5.56943	-1.84764	2.838783
C9	-4.77064	-2.72744	2.111094
C10	-3.60824	-2.25792	1.508271
C11	-3.2173	-0.91902	1.614932
C12	-4.03528	-0.05781	2.354953
C13	-5.20256	-0.50891	2.962479
F14	-6.68417	-2.28749	3.418761
F15	-5.1181	-4.0116	2.003826
F16	-2.85506	-3.12814	0.825328
F17	-3.71179	1.232109	2.486787
F18	-5.97233	0.331794	3.656554
C19	-0.26393	0.114373	5.764201
C20	-0.32198	-1.06954	5.032607
C21	-0.59044	-1.02281	3.669358
C22	-0.81856	0.187744	2.995694
C23	-0.76499	1.35766	3.764291

C24	-0.48714	1.332161	5.126386
F25	-0.00428	0.082036	7.072827
F26	-0.11207	-2.24038	5.640829
F27	-0.63124	-2.17404	2.980934
F28	-1.02086	2.546752	3.190557
F29	-0.45105	2.469199	5.827995
C30	-4.16452	-1.58646	-3.51719
C31	-4.52847	-0.57082	-2.63679
C32	-3.70081	-0.25449	-1.56461
C33	-2.50681	-0.95249	-1.33006
C34	-2.1678	-1.9702	-2.23205
C35	-2.97647	-2.28673	-3.31706
F36	-4.95374	-1.89121	-4.5495
F37	-5.66538	0.104201	-2.83177
F38	-4.06585	0.737648	-0.74263
F39	-1.03384	-2.66364	-2.04358
F40	-2.63255	-3.26728	-4.15608
H41	1.440498	0.857938	-2.41817
H42	2.597211	0.513213	0.928138
O43	3.299512	2.52227	-1.33191
O44	3.383979	-2.3221	-2.24378
O45	4.659869	0.097971	-1.27091
H46	2.474918	1.714088	-0.14107
H47	3.726498	3.291611	-0.93256
H48	2.819977	-2.4462	-1.4668
H49	3.880783	-1.51241	-2.03441
H50	5.588115	0.188278	-1.51701
O51	1.250861	-1.66623	-0.10064
O52	-0.5599	2.034981	-0.68348
H53	0.574157	-2.35786	-0.14614
H54	4.099232	-0.62187	0.390244
O55	3.500008	-0.74458	1.153737
H56	2.813812	-1.3723	0.841684
H57	1.158697	-0.95776	-1.23933
H58	2.449405	2.868503	-1.79712
O59	1.049158	3.22191	-2.30329
H60	0.363347	2.744758	-1.70325
H61	-0.39334	2.622738	0.079814
O62	0.774849	3.680896	1.257332
H63	1.282585	2.850984	1.307455

H64	0.252441	3.690403	2.06936
H65	0.827526	4.159957	-2.25402
C66	0.977613	-0.11233	-2.26367
H67	0.039233	-0.18613	-2.81026

Table S91. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_3{}^{eq}\text{-}H\text{-}OH^{ax})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.250494	0.275545	-0.2796
N2	-0.95645	0.283739	1.541902
H3	3.514939	0.337931	-0.49486
C4	-1.94054	-0.36874	0.928564
O5	2.049953	1.147809	0.276208
N6	-1.67466	-0.55956	-0.36037
H7	1.823278	-0.85992	-2.64061
C8	-5.46689	-1.81556	2.909727
C9	-4.67831	-2.69085	2.165135
C10	-3.54138	-2.20995	1.52462
C11	-3.16574	-0.86572	1.609962
C12	-3.97031	-0.00994	2.369139
C13	-5.11375	-0.47117	3.013574
F14	-6.55835	-2.26517	3.525205
F15	-5.01108	-3.98024	2.077305
F16	-2.7954	-3.0746	0.825923
F17	-3.6562	1.2842	2.483933
F18	-5.87384	0.364385	3.72429
C19	-0.06354	-0.00683	5.655705
C20	-0.18956	-1.1615	4.886773
C21	-0.50571	-1.05729	3.537564
C22	-0.71621	0.181829	2.91141
C23	-0.58496	1.320664	3.716279
C24	-0.26201	1.239121	5.066018
F25	0.239314	-0.09315	6.952189
F26	0.001037	-2.35911	5.445743
F27	-0.60795	-2.18317	2.81259
F28	-0.79761	2.543496	3.190335
F29	-0.15715	2.3501	5.801404
C30	-4.32889	-1.63521	-3.44191
C31	-4.67125	-0.60448	-2.57023
C32	-3.80313	-0.24979	-1.54297
C33	-2.58734	-0.92018	-1.34413

C34	-2.27105	-1.95188	-2.23806
C35	-3.1201	-2.30945	-3.27821
F36	-5.15681	-1.97789	-4.43103
F37	-5.82598	0.048779	-2.73119
F38	-4.1445	0.761965	-0.73229
F39	-1.11529	-2.62117	-2.08392
F40	-2.79422	-3.30283	-4.10882
H41	1.494257	0.857597	-2.48208
H42	2.357417	0.576895	1.020642
O43	2.885902	3.510055	-0.93057
O44	3.355056	-2.3899	-2.17865
O45	4.29678	-0.25493	-0.585
H46	2.789577	2.605574	-0.55955
H47	2.483538	4.048946	-0.23006
H48	2.784941	-2.73435	-1.47834
H49	3.848496	-1.68464	-1.71821
H50	5.044345	0.313639	-0.80663
O51	1.099673	-1.62255	-0.13836
O52	-0.53455	2.184741	-0.69948
H53	0.355474	-2.23847	-0.23274
H54	3.755192	-0.91888	1.280973
O55	2.968012	-0.91762	1.853377
H56	2.324045	-1.43908	1.337813
H57	1.182653	-0.98092	-1.31181
H58	1.687704	3.433629	-2.12098
O59	0.874698	3.221813	-2.65691
H60	-0.09816	2.554706	-1.52538
H61	-0.17943	2.762709	0.028964
O62	0.960684	3.418459	1.127154
H63	1.438888	2.54838	1.032834
H64	0.570631	3.428578	2.010982
H65	0.585005	4.046243	-3.06504
C66	1.051656	-0.12385	-2.33079
H67	0.163354	-0.26768	-2.94436

Table S92. $[Rh^{III}(NN^{F})(OH)_2(CH_3{}^{eq}\text{-}H\text{-}OH^{ax})]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.307098	0.050339	-0.33239
N2	-0.93508	0.071201	1.415119
H3	3.387986	0.165207	0.678488

C4	-1.96703	-0.48971	0.798373
O5	2.042371	0.94578	0.220404
N6	-1.67159	-0.75663	-0.47786
H7	2.455784	-0.35513	-2.3697
C8	-5.7763	-1.3262	2.617735
C9	-5.12324	-2.31321	1.884775
C10	-3.89238	-2.03321	1.301067
C11	-3.28567	-0.77956	1.428247
C12	-3.96632	0.193982	2.166479
C13	-5.19679	-0.0687	2.761146
F14	-6.95873	-1.58605	3.182498
F15	-5.67735	-3.52431	1.753743
F16	-3.28725	-3.01267	0.619425
F17	-3.45044	1.41913	2.311297
F18	-5.82987	0.881227	3.459084
C19	0.137086	0.102737	5.482377
C20	-0.51536	-1.006	4.957448
C21	-0.89454	-1.01735	3.621727
C22	-0.66269	0.07562	2.772133
C23	0.021592	1.167101	3.32783
C24	0.415119	1.189116	4.658256
F25	0.495943	0.1264	6.773438
F26	-0.76542	-2.06659	5.738585
F27	-1.4613	-2.13778	3.136299
F28	0.321913	2.221943	2.552803
F29	1.049291	2.257518	5.160231
C30	-4.30871	-1.1857	-3.72947
C31	-4.52875	-0.1772	-2.7969
C32	-3.66955	-0.04154	-1.71296
C33	-2.58664	-0.91057	-1.50509
C34	-2.38343	-1.90614	-2.47345
C35	-3.22603	-2.04712	-3.56943
F36	-5.13233	-1.32669	-4.77662
F37	-5.55627	0.668203	-2.95634
F38	-3.87589	0.978454	-0.85808
F39	-1.34993	-2.75042	-2.34294
F40	-3.0152	-3.0189	-4.46653
H42	0.956898	0.527391	-2.62958
H43	1.747926	1.590298	0.87956
O44	2.933998	2.592107	-1.73758

O46	4.83695	0.377871	-1.95644
O47	4.269072	-0.24818	0.91932
H48	2.584075	1.934545	-1.08492
H49	2.580571	3.428548	-1.37357
H52	4.713113	0.063417	-1.04409
H53	4.391582	1.241675	-1.97248
H54	4.778866	0.484843	1.287318
O55	1.181546	-1.86891	-0.09639
O56	-0.35852	1.915013	-0.82468
H56	0.469357	-2.49315	-0.30326
H57	-1.26924	1.991796	-0.51006
H59	3.061376	-1.17554	2.266104
O60	2.205557	-1.52797	2.564414
H61	1.805963	-1.77799	1.711432
H64	1.374719	-1.23833	-1.23142
H65	1.434005	2.722051	-2.99276
O66	0.509191	2.917669	-3.247
H67	0.016952	2.503977	-2.50407
H68	0.531654	3.571365	-0.54649
O69	0.967016	4.400327	-0.84265
H70	0.741918	4.362373	-1.79096
C70	1.363314	-0.4324	-2.30601
H71	0.953718	-1.19687	-2.97631

Table S93. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{ax})(CH_3{}^{eq}\text{-}H\text{-}OH^{eq})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.148706	0.261735	-0.23074
N2	-1.03225	0.195677	1.566971
H3	4.424063	-2.02242	-0.13179
C4	-2.01903	-0.46466	0.964235
O5	1.996099	1.268318	-0.03944
N6	-1.73606	-0.65987	-0.32028
H7	2.141426	-0.3956	-2.41207
C8	-5.56929	-1.82873	2.962267
C9	-4.84422	-2.70643	2.158803
C10	-3.69759	-2.25585	1.51312
C11	-3.24985	-0.93735	1.648968
C12	-3.99456	-0.07805	2.465618
C13	-5.14514	-0.51029	3.116835
F14	-6.66825	-2.25056	3.5839

F15	-5.24614	-3.97161	2.019924
F16	-3.01576	-3.12578	0.758967
F17	-3.61888	1.194132	2.628324
F18	-5.84527	0.329775	3.881905
C19	0.106848	-0.20902	5.605398
C20	-0.15648	-1.34307	4.840971
C21	-0.5507	-1.20108	3.516563
C22	-0.7154	0.056666	2.914193
C23	-0.44154	1.1745	3.712715
C24	-0.03394	1.054159	5.035987
F25	0.485939	-0.3313	6.878561
F26	-0.01923	-2.55803	5.378648
F27	-0.77724	-2.31427	2.792855
F28	-0.59526	2.412708	3.205652
F29	0.20626	2.14517	5.768469
C30	-4.41075	-1.37703	-3.4923
C31	-4.73668	-0.43803	-2.5176
C32	-3.85978	-0.20103	-1.46468
C33	-2.65279	-0.90644	-1.33558
C34	-2.34828	-1.83747	-2.33893
C35	-3.20695	-2.0732	-3.40621
F36	-5.247	-1.60786	-4.50682
F37	-5.88278	0.244517	-2.60506
F38	-4.18495	0.737383	-0.56308
F39	-1.1958	-2.52016	-2.27502
F40	-2.89183	-2.97372	-4.34145
H42	0.991517	0.923408	-2.92065
H43	2.538201	0.69787	0.601686
O44	2.427964	3.791077	-1.34874
O47	5.060271	-1.68534	0.545268
H48	2.590821	2.884728	-1.02341
H49	2.026027	4.211617	-0.57007
H53	1.727991	0.64647	-1.16498
H54	5.636244	-1.08105	0.061135
O55	1.060756	-1.46365	0.338823
O56	-0.7983	2.109977	-0.72785
H57	0.369348	-2.08559	0.602752
H58	3.870325	-0.7549	1.46122
O59	3.04699	-0.29575	1.755138
H60	2.326869	-0.91745	1.509291

H61	2.95209	-3.27324	-1.42486
O62	3.078812	-2.34961	-1.17748
H63	2.270924	-2.09156	-0.65499
H64	1.124396	3.529748	-2.4081
O65	0.281843	3.236923	-2.85074
H66	-0.47991	2.484382	-1.60153
H67	-0.42941	2.735495	-0.0545
O68	0.815431	3.480396	0.941389
H69	1.346827	2.657422	0.802617
H70	0.553268	3.476691	1.87123
H71	-0.13681	4.033088	-3.19924
C71	1.162701	0.076495	-2.25492
H72	0.443693	-0.71681	-2.45845

Table S94. $[Rh^{III}(NN^{F})(OH)_2(CH_3^{eq}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.360345	-0.0096	-0.24342
N2	-0.74772	-0.21556	1.632722
H3	3.046642	0.846367	1.443075
C4	-1.80777	-0.69836	1.008166
O5	2.213358	1.007262	-0.17907
N6	-1.56627	-0.86175	-0.29676
H7	1.929504	0.494656	-2.84162
C8	-5.60438	-1.54693	2.844085
C9	-4.99209	-2.50549	2.040875
C10	-3.76297	-2.22484	1.453107
C11	-3.11969	-0.99903	1.647963
C12	-3.75903	-0.05302	2.45553
C13	-4.98727	-0.31657	3.053944
F14	-6.78494	-1.8072	3.412107
F15	-5.58499	-3.68866	1.844267
F16	-3.19872	-3.1714	0.696629
F17	-3.20376	1.145213	2.665416
F18	-5.58177	0.606305	3.818686
C19	0.223737	-0.57483	5.712567
C20	-0.35993	-1.64568	5.044796
C21	-0.69689	-1.52216	3.705148
C22	-0.49318	-0.33246	2.989913
C23	0.113754	0.718175	3.687078
C24	0.470124	0.608559	5.024268

F25	0.543496	-0.68006	7.009566
F26	-0.57934	-2.79777	5.693276
F27	-1.19444	-2.60077	3.073586
F28	0.394483	1.869822	3.047682
F29	1.041532	1.643474	5.656032
C30	-4.3834	-0.75258	-3.42502
C31	-4.42315	0.216923	-2.42714
C32	-3.50366	0.168462	-1.38646
C33	-2.53761	-0.84549	-1.28962
C34	-2.52443	-1.80576	-2.31163
C35	-3.42834	-1.76417	-3.36756
F36	-5.26507	-0.71832	-4.43177
F37	-5.33689	1.19432	-2.48118
F38	-3.5483	1.132906	-0.44923
F39	-1.63855	-2.81009	-2.27026
F40	-3.40172	-2.70468	-4.31974
H42	0.192546	0.406457	-2.81873
H43	1.83966	1.903671	-0.12156
O44	2.699256	3.152366	-2.41749
O47	3.266782	0.940458	2.393711
H48	3.071952	2.431242	-1.89238
H49	2.217087	3.69826	-1.75646
H52	1.745317	0.543884	-1.33061
H54	2.536158	1.475139	2.729231
O55	1.226679	-1.8465	0.057209
O56	-0.38471	1.910073	-0.55322
H56	0.510883	-2.40428	0.395097
H57	-1.19231	1.994173	-0.03047
H59	2.729246	-0.89923	2.731266
O60	2.261693	-1.75262	2.695876
H61	2.035851	-1.83484	1.746358
H62	0.520368	-3.3408	-2.42752
O63	1.468142	-3.34791	-2.2474
H64	1.525354	-2.8378	-1.40427
H65	0.744279	2.944183	-3.14122
O66	-0.21534	3.085312	-3.0542
H67	-0.43265	2.571025	-2.24352
H68	0.409699	3.545963	-0.4256
O69	0.811358	4.379547	-0.76497
H70	0.3459	4.429669	-1.62263

C70	1.081578	-0.02506	-2.36278
H71	1.209185	-1.0923	-2.53441

Table S95. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 7H_2O$

Atom	x	y	z
Rh1	0.120036	0.70012	-0.12502
N2	-1.03812	0.50022	1.590346
H3	3.930403	-0.56842	0.258284
C4	-2.11818	0.074832	0.930329
O5	1.840333	1.728475	0.538629
N6	-1.84945	0.005282	-0.36819
H7	1.587866	0.024066	-2.25418
C8	-5.93942	-0.81015	2.670924
C9	-5.32702	-1.73844	1.830425
C10	-4.08359	-1.44743	1.280087
C11	-3.4293	-0.24066	1.548339
C12	-4.06499	0.672743	2.396299
C13	-5.30822	0.399307	2.956772
F14	-7.12945	-1.07945	3.201682
F15	-5.93007	-2.89816	1.564151
F16	-3.51227	-2.3584	0.484693
F17	-3.488	1.847149	2.674493
F18	-5.9002	1.288457	3.755816
C19	-0.1995	0.079083	5.69085
C20	-0.68681	-1.00975	4.971237
C21	-0.96517	-0.86717	3.617111
C22	-0.79734	0.355153	2.949769
C23	-0.291	1.42772	3.696412
C24	0.006961	1.298425	5.048351
F25	0.074651	-0.04673	6.990359
F26	-0.86576	-2.18683	5.577559
F27	-1.38727	-1.94247	2.927529
F28	-0.08834	2.609772	3.101135
F29	0.476108	2.340645	5.738458
C30	-4.55566	-0.07149	-3.58781
C31	-4.70011	0.886056	-2.58716
C32	-3.81588	0.895949	-1.51645
C33	-2.78449	-0.04606	-1.39856
C34	-2.66232	-0.99396	-2.42187
C35	-3.53058	-1.01097	-3.50675

F36	-5.39993	-0.09165	-4.62062
F37	-5.67541	1.7955	-2.66718
F38	-3.94518	1.851536	-0.57945
F39	-1.69263	-1.91844	-2.35857
F40	-3.39634	-1.93377	-4.46359
O41	0.866858	0.760532	-2.08395
H42	1.40896	1.564978	-2.33051
H43	2.081423	1.207429	1.330284
O44	4.053812	2.316901	-0.81978
O45	2.756639	2.174668	-3.22035
O46	2.779248	-0.77404	-2.63712
O47	4.453329	-0.45768	-0.56297
H48	3.213945	2.166466	-0.30801
H49	4.481999	3.087295	-0.4274
H50	3.350509	2.407487	-2.47426
H51	3.070002	1.298042	-3.49806
H52	2.379955	-1.68021	-2.62065
H53	3.427994	-0.74041	-1.87825
H54	4.593767	0.505699	-0.62462
O55	0.765417	-1.30501	0.057136
H56	0.0545	-1.77397	0.517558
H57	2.917775	-1.24252	2.331293
O58	2.690018	-0.60359	1.645561
H59	1.960316	-1.01502	1.075819
H60	0.422172	-2.80845	-2.62506
O61	1.226917	-2.88262	-2.09677
H62	1.028964	-2.35555	-1.27907
H63	-0.219	3.639064	0.629848
H64	-1.48948	2.701555	-0.1104
H65	0.690617	2.356431	0.374499
C66	-0.42688	2.939597	-0.19791
O67	-0.05903	3.544395	-1.39634
H68	-0.56079	3.118287	-2.12483
O69	-1.19873	1.997405	-3.41004
H70	-0.52154	1.339107	-3.14952
H71	-0.87737	2.371537	-4.24109

Table S96. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.206593	0.500162	0.119626

N2	-0.97044	0.062051	1.80088
H3	4.044831	1.147123	-1.493
C4	-2.0121	-0.36234	1.091107
O5	1.806508	1.489429	1.006271
N6	-1.75643	-0.28376	-0.21357
H7	0.997638	2.123992	-2.36199
C8	-5.74928	-1.64962	2.773838
C9	-5.09055	-2.45794	1.849346
C10	-3.87974	-2.03668	1.30973
C11	-3.30069	-0.81742	1.675552
C12	-3.98265	-0.02554	2.606092
C13	-5.1959	-0.42879	3.154361
F14	-6.91044	-2.04388	3.292945
F15	-5.61989	-3.63016	1.491678
F16	-3.26708	-2.83545	0.43016
F17	-3.48247	1.156851	2.981533
F18	-5.8334	0.348811	4.032185
C19	-0.04503	-0.80937	5.815043
C20	-0.51566	-1.82079	4.982323
C21	-0.8313	-1.53409	3.659147
C22	-0.71445	-0.2365	3.134657
C23	-0.22889	0.758465	3.995723
C24	0.105131	0.482494	5.316527
F25	0.260812	-1.07635	7.086803
F26	-0.64894	-3.06537	5.452559
F27	-1.24658	-2.53699	2.871083
F28	-0.08768	2.011902	3.549924
F29	0.553221	1.454931	6.115908
C30	-4.60547	-0.28393	-3.32301
C31	-4.73648	0.608332	-2.26155
C32	-3.79894	0.598177	-1.2349
C33	-2.7211	-0.30138	-1.21438
C34	-2.61981	-1.18335	-2.29899
C35	-3.53882	-1.17941	-3.34204
F36	-5.49614	-0.28101	-4.31695
F37	-5.75032	1.478283	-2.24187
F38	-3.92628	1.492115	-0.23966
F39	-1.62201	-2.0836	-2.33451
F40	-3.41151	-2.04335	-4.35437
O41	1.041977	0.734227	-1.76282

H42	2.00818	0.605664	-1.6108
H43	2.336072	1.941951	0.312662
O44	3.3417	2.904423	-1.03564
O45	1.104034	3.125979	-2.56285
O46	3.741417	-1.36889	-3.61874
O47	3.769771	0.215295	-1.44387
H48	3.639542	3.718914	-0.61309
H49	2.625607	3.163178	-1.66283
H50	0.975543	3.27203	-3.50696
H51	2.802806	-1.60395	-3.43857
H52	4.239612	-2.17362	-3.42837
H53	3.947831	-0.25163	-2.29635
O54	0.925011	-1.54397	0.089441
H55	-1.43583	2.401019	-0.11998
H56	-0.78302	2.979181	1.418939
H57	0.594893	2.114684	0.78468
H58	1.859065	-1.44622	0.467478
H59	1.023828	-1.80615	-0.85371
O60	3.260866	-0.87633	1.030655
H61	2.877259	-0.02939	1.342207
H62	3.677842	-0.60101	0.18617
O63	1.173122	-1.68364	-2.68915
H64	0.984776	-0.71278	-2.49026
H65	0.362693	-2.04343	-3.07127
C66	-0.52688	2.74181	0.381957
O67	0.077313	3.852516	-0.20281
H68	0.231719	3.694451	-1.15874

Table S97. $[Rh^{III}(NN^{F})(OH)_2(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{-‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	-0.03661	0.594054	-0.1062
N2	-0.93883	0.19949	1.812799
H3	5.101292	0.091877	0.923812
C4	-2.12502	-0.03492	1.26026
O5	1.893405	1.367122	0.341573
N6	-2.07684	0.141786	-0.05738
H7	1.369327	1.778934	-2.54661
C8	-5.66664	-1.12826	3.449932
C9	-5.26352	-1.88851	2.356115
C10	-4.11876	-1.52815	1.651331

C11	-3.3542	-0.41511	2.014007
C12	-3.78557	0.332973	3.114068
C13	-4.92672	-0.01281	3.831213
F14	-6.76503	-1.46818	4.133156
F15	-5.97372	-2.96524	1.995345
F16	-3.75785	-2.28854	0.614521
F17	-3.11047	1.420829	3.50189
F18	-5.32257	0.724573	4.877037
C19	0.554355	-1.05659	5.543522
C20	-0.22871	-1.92607	4.793426
C21	-0.74226	-1.51733	3.568219
C22	-0.51605	-0.22749	3.059
C23	0.28856	0.620932	3.837526
C24	0.818765	0.219671	5.0565
F25	1.048002	-1.44362	6.729754
F26	-0.47641	-3.1638	5.250889
F27	-1.45606	-2.40733	2.858622
F28	0.560649	1.857426	3.402071
F29	1.57124	1.062931	5.778992
C30	-5.24422	0.818136	-2.74431
C31	-5.21826	1.490266	-1.52729
C32	-4.17503	1.261048	-0.63813
C33	-3.14627	0.343286	-0.90939
C34	-3.19014	-0.30557	-2.15547
C35	-4.22168	-0.07265	-3.05919
F36	-6.24862	1.02672	-3.60928
F37	-6.18847	2.36725	-1.22473
F38	-4.14945	1.97093	0.505721
F39	-2.24334	-1.18288	-2.48341
F40	-4.25321	-0.72303	-4.23194
O41	0.29188	0.907704	-2.08978
H42	0.530611	0.030492	-2.44235
H43	2.400508	1.075054	-0.45547
O44	2.554872	4.068762	-0.86325
O45	2.218963	2.300399	-2.89371
O46	3.475602	0.240232	-1.68405
O47	4.985835	-0.70145	0.385946
H48	2.531568	3.51904	-1.68432
H49	2.657864	3.397316	-0.17101
H50	1.992099	2.62718	-3.77183

H51	2.87927	-0.50267	-1.98486
H52	3.31383	0.964449	-2.32413
H53	4.571325	-0.35847	-0.43834
O54	0.402308	-1.45226	-0.25793
H55	0.020711	3.27724	1.194936
H57	0.906253	2.133709	0.185092
H58	1.069729	-1.5478	0.450893
O59	2.49556	-0.99828	1.763081
H60	2.27395	-0.09282	1.470931
H61	3.347212	-1.15407	1.308022
O62	1.642956	-1.52981	-2.38559
H63	1.72337	-2.42128	-2.74123
H64	1.108377	-1.59109	-1.45337
C65	-0.3261	2.891068	0.217176
H66	-1.38363	2.661235	0.349817
O66	-0.20983	3.826509	-0.81969
H67	0.736825	4.080365	-0.87565

Table S98. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.296291	0.106618	-0.16125
N2	-0.87703	-0.06807	1.646052
H3	3.635505	0.293357	0.174126
C4	-1.91215	-0.57388	0.995585
O5	2.094798	0.886551	0.507856
N6	-1.634	-0.70977	-0.30884
C8	-5.65019	-1.70481	2.786239
C9	-4.9637	-2.60872	1.977853
C10	-3.75437	-2.23155	1.404954
C11	-3.20639	-0.9624	1.614834
C12	-3.91579	-0.07442	2.429816
C13	-5.12571	-0.43429	3.015068
F14	-6.80844	-2.05633	3.341189
F15	-5.46263	-3.82861	1.765465
F16	-3.10724	-3.12735	0.648052
F17	-3.44504	1.156147	2.656644
F18	-5.78767	0.431487	3.785785
C19	0.016866	-0.09046	5.756976
C20	-0.49847	-1.23762	5.160456
C21	-0.81254	-1.22944	3.806915

C22	-0.65103	-0.08276	3.012761
C23	-0.11175	1.050455	3.639676
C24	0.21813	1.05413	4.989081
F25	0.320794	-0.08847	7.057348
F26	-0.67521	-2.34679	5.88572
F27	-1.2548	-2.36897	3.247242
F28	0.101554	2.165234	2.92317
F29	0.71853	2.156813	5.557343
C30	-4.24277	-1.28746	-3.56394
C31	-4.57436	-0.36012	-2.57986
C32	-3.72628	-0.16479	-1.49434
C33	-2.54151	-0.90191	-1.34122
C34	-2.23459	-1.82129	-2.35561
C35	-3.06067	-2.01732	-3.45437
F36	-5.05039	-1.47375	-4.61002
F37	-5.69773	0.35526	-2.69114
F38	-4.05325	0.768382	-0.58826
F39	-1.09655	-2.53918	-2.26917
F40	-2.73695	-2.90756	-4.39585
H41	0.340293	0.717532	-2.60822
H42	2.1716	0.415661	1.365038
O43	2.138306	3.250881	-2.30984
O44	3.744486	-1.72438	-1.86321
O45	4.473658	-0.24434	0.26876
H46	2.436514	2.32046	-2.37517
H47	2.132506	3.458118	-1.35516
H48	3.022372	-2.16802	-1.39046
H49	4.24737	-1.29914	-1.13194
H50	5.208072	0.380282	0.300955
O51	1.192191	-1.79252	-0.30306
O52	-0.5502	2.030014	-0.28724
H53	0.454438	-2.40585	-0.45373
H54	3.508324	-1.11778	1.84453
O55	2.62034	-1.23091	2.22747
H56	2.135925	-1.68692	1.517246
H57	1.153958	-0.99449	-1.33055
H58	0.557868	3.114902	-2.70654
O59	-0.41601	2.866831	-2.75534
H60	-0.61387	2.345155	-1.24077
H61	0.105476	2.651609	0.13056

O62	1.607054	3.367429	0.461659
H63	1.925651	2.410149	0.619975
H64	1.711299	3.859687	1.28441
H65	-0.89778	3.660322	-3.01746
C66	1.082921	-0.03059	-2.33434
H67	0.846738	-0.92108	-2.94828
O67	2.364676	0.458358	-2.57607
H68	2.999772	-0.28997	-2.41598

Table S99. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.267277	0.282655	-0.15904
N2	-1.01182	0.311201	1.640931
H3	3.683766	-0.01207	-2.0501
C4	-1.93441	-0.38558	0.992525
O5	2.016776	1.269881	0.546431
N6	-1.58706	-0.60169	-0.27819
H7	1.259609	-1.17777	-2.67585
C8	-5.49725	-1.96562	2.798676
C9	-4.64763	-2.80655	2.082573
C10	-3.50006	-2.28234	1.497232
C11	-3.17363	-0.9266	1.61015
C12	-4.04134	-0.1054	2.338216
C13	-5.19487	-0.6112	2.928618
F14	-6.59846	-2.45744	3.362011
F15	-4.93242	-4.10533	1.969328
F16	-2.69717	-3.11623	0.825661
F17	-3.77978	1.198127	2.474531
F18	-6.01283	0.191645	3.612284
C19	-0.37528	0.171706	5.809093
C20	-0.36459	-1.00428	5.062485
C21	-0.59816	-0.9517	3.693218
C22	-0.85388	0.256782	3.024863
C23	-0.86413	1.418718	3.807665
C24	-0.62808	1.387037	5.177683
F25	-0.15351	0.133574	7.124286
F26	-0.12542	-2.1734	5.662557
F27	-0.57912	-2.09702	2.993723
F28	-1.1419	2.607243	3.240188
F29	-0.65953	2.516038	5.892267

C30	-4.09698	-1.4818	-3.53849
C31	-4.4772	-0.50237	-2.6244
C32	-3.65663	-0.21073	-1.5398
C33	-2.45294	-0.89908	-1.32346
C34	-2.09685	-1.87737	-2.26216
C35	-2.89774	-2.16931	-3.35968
F36	-4.87849	-1.76116	-4.58362
F37	-5.62119	0.1657	-2.8004
F38	-4.03579	0.754266	-0.69133
F39	-0.94709	-2.5521	-2.09861
F40	-2.53512	-3.11192	-4.23261
H42	2.735459	0.582904	0.768895
O43	2.782344	3.513908	-0.58435
O44	2.774014	-2.86835	-2.28571
O45	4.404478	-0.58511	-1.69308
H46	2.405927	2.007148	-0.01766
H47	2.285144	4.009986	0.088594
H48	2.414043	-2.8231	-1.38835
H49	3.528083	-2.25486	-2.24283
H50	5.231035	-0.2608	-2.06977
O51	1.237526	-1.61694	0.03582
O52	-0.52597	2.064657	-0.74536
H53	0.524993	-2.27365	0.01392
H54	4.113713	-0.70171	0.093795
O55	3.643053	-0.67486	0.955378
H56	2.91133	-1.31375	0.843117
H57	1.180105	-0.90884	-1.15564
H58	2.217782	3.56787	-1.38714
O59	0.985224	2.975875	-2.51006
H60	0.275902	2.6418	-1.80422
H61	-0.37653	2.66501	0.009676
O62	0.770126	3.585353	1.380229
H63	1.195221	2.716299	1.504379
H64	0.236599	3.731873	2.170806
H65	0.529046	3.410454	-3.23954
C66	1.067337	-0.16604	-2.27498
H67	0.131848	0.197443	-2.70375
O67	2.168519	0.637871	-2.58766
H68	1.842558	1.575283	-2.66398

Table S100. $[Rh^{III}(NN^{F})(OH)_2(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{-‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.351518	-0.00142	-0.31993
N2	-0.92166	0.039147	1.469363
H3	3.506298	0.208232	0.544713
C4	-1.94467	-0.5054	0.829379
O5	2.108491	0.903675	0.182911
N6	-1.63464	-0.77957	-0.44435
C8	-5.82481	-1.28897	2.525327
C9	-5.16237	-2.28383	1.811653
C10	-3.90862	-2.02119	1.270361
C11	-3.28686	-0.77732	1.420271
C12	-3.97794	0.204101	2.137452
C13	-5.23089	-0.04122	2.691343
F14	-7.02922	-1.53204	3.050257
F15	-5.73036	-3.48608	1.657736
F16	-3.29734	-3.00969	0.607054
F17	-3.45036	1.421184	2.302209
F18	-5.87162	0.917027	3.371107
C19	0.073507	0.103855	5.558583
C20	-0.6254	-0.98153	5.044565
C21	-0.97967	-1.00633	3.701605
C22	-0.67891	0.052845	2.828472
C23	0.053538	1.119053	3.376613
C24	0.422795	1.153153	4.713532
F25	0.409855	0.139106	6.85597
F26	-0.94645	-2.00944	5.844426
F27	-1.59397	-2.1111	3.236104
F28	0.427424	2.138486	2.585813
F29	1.106144	2.198042	5.200706
C30	-4.27945	-1.13939	-3.70185
C31	-4.4601	-0.11203	-2.78151
C32	-3.59679	0.001998	-1.69835
C33	-2.54939	-0.90689	-1.4777
C34	-2.38574	-1.92061	-2.43456
C35	-3.23231	-2.04118	-3.53018
F36	-5.10674	-1.2595	-4.74869
F37	-5.45376	0.770692	-2.95223
F38	-3.76502	1.038202	-0.85416
F39	-1.38534	-2.80263	-2.29451

F40	-3.0599	-3.03152	-4.41485
H42	1.140189	0.542138	-2.68651
H43	1.840578	1.447443	0.937477
O44	2.865335	2.71009	-1.64353
O46	4.666093	0.664579	-2.02492
O47	4.445882	-0.10231	0.733079
H48	2.524302	2.025919	-1.00705
H49	2.44753	3.528158	-1.30137
H52	4.76155	0.356527	-1.10032
H53	4.280278	1.560134	-1.95231
H54	4.832541	0.625175	1.237779
O55	1.211438	-1.91832	-0.11307
O56	-0.32323	1.862054	-0.84906
H56	0.483454	-2.54196	-0.25295
H57	-1.24897	1.920885	-0.57744
H59	3.205949	-1.13609	2.113671
O60	2.346911	-1.43703	2.450433
H61	1.911033	-1.72025	1.623916
H64	1.257172	-1.20552	-1.28451
H65	1.41843	2.793316	-2.98934
O66	0.486961	2.925225	-3.25339
H67	0.022471	2.469445	-2.51508
H68	0.435607	3.550866	-0.54068
O69	0.82386	4.40947	-0.82443
H70	0.600211	4.37312	-1.77315
C70	1.330684	-0.50756	-2.45793
H71	0.616367	-1.13317	-3.00682
O67	2.618792	-0.94318	-2.73625
H69	3.309373	-0.27093	-2.48764

Table S101. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{ax})(CH_2OH^{eq}\text{-}H\text{-}OH^{eq})]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.211178	0.184806	-0.1032
N2	-0.96738	-0.06415	1.643002
H3	4.528172	-1.97436	0.149082
C4	-1.99013	-0.60001	0.997889
O5	2.056263	1.091536	0.251769
N6	-1.69634	-0.71919	-0.30354
H7	2.332961	-0.31425	-2.25013
C8	-5.69977	-1.80187	2.801507

C9	-5.02832	-2.67262	1.945687
C10	-3.8269	-2.27515	1.369386
C11	-3.27192	-1.01638	1.621868
C12	-3.96676	-0.1619	2.485142
C13	-5.16792	-0.5433	3.074316
F14	-6.85054	-2.17311	3.359041
F15	-5.53414	-3.88151	1.690648
F16	-3.19631	-3.14101	0.56601
F17	-3.49271	1.058514	2.755404
F18	-5.81524	0.291615	3.890193
C19	0.137439	-0.20125	5.69604
C20	-0.4121	-1.33169	5.098023
C21	-0.79878	-1.2875	3.764094
C22	-0.67782	-0.11905	2.995151
C23	-0.10706	0.997863	3.622894
C24	0.296939	0.96489	4.950898
F25	0.511074	-0.23522	6.977225
F26	-0.5516	-2.46014	5.801552
F27	-1.27515	-2.41129	3.199661
F28	0.060384	2.131359	2.925637
F29	0.828025	2.051282	5.520809
C30	-4.31061	-1.07404	-3.58875
C31	-4.63933	-0.21589	-2.5432
C32	-3.78796	-0.09603	-1.44969
C33	-2.60284	-0.8433	-1.34714
C34	-2.29558	-1.68918	-2.4248
C35	-3.12734	-1.80788	-3.53154
F36	-5.12079	-1.18818	-4.64387
F37	-5.76162	0.508966	-2.60314
F38	-4.11199	0.780688	-0.48638
F39	-1.15781	-2.4017	-2.3947
F40	-2.8063	-2.62982	-4.53487
H43	2.482091	0.484106	0.93569
O44	1.499482	4.072744	-2.25611
O47	5.046623	-1.74859	0.958292
H48	1.877868	3.201932	-2.48178
H49	1.560548	4.118005	-1.28009
H53	1.819455	0.582114	-0.95258
H54	5.633503	-1.03429	0.681269
O55	1.087425	-1.62132	0.2086

O56	-0.75476	2.084917	-0.28094
H57	0.379552	-2.2753	0.126083
H58	3.685758	-1.03882	1.845113
O59	2.812665	-0.64156	2.077501
H60	2.158698	-1.24443	1.666139
H61	3.296945	-3.04925	-1.50665
O62	3.336783	-2.16883	-1.11434
H63	2.462669	-2.03114	-0.65325
H64	-0.02178	3.614413	-2.64545
O65	-0.81638	3.010423	-2.77923
H66	-0.90653	2.392475	-1.2108
H67	-0.13757	2.74862	0.121938
O68	1.337605	3.552375	0.481559
H69	1.77426	2.644188	0.508846
H70	1.420016	3.937522	1.362318
H71	-1.51786	3.514041	-3.20787
C71	1.354049	0.176597	-2.14926
H72	0.626095	-0.58282	-2.44461
O67	1.337788	1.320713	-2.97847
H68	0.420658	1.608435	-3.13367

Table S102. $[Rh^{III}(NN^{F})(OH)_2(CH_2OH^{eq}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.353848	-0.00652	-0.31647
N2	-0.7111	-0.22248	1.657037
H3	3.000382	0.412702	1.233826
C4	-1.79104	-0.6584	1.034118
O5	2.30084	0.803288	-0.41384
N6	-1.58917	-0.78698	-0.27748
H7	1.538075	0.722238	-3.02468
C8	-5.60838	-1.41151	2.871567
C9	-4.99748	-2.40459	2.110479
C10	-3.76094	-2.15655	1.524078
C11	-3.10872	-0.93112	1.680442
C12	-3.74611	0.049607	2.444967
C13	-4.98261	-0.17961	3.040867
F14	-6.79688	-1.64081	3.43807
F15	-5.59993	-3.5894	1.952723
F16	-3.19773	-3.13321	0.805519
F17	-3.17929	1.250013	2.613827

F18	-5.57635	0.777133	3.764326
C19	0.173732	-0.51683	5.7643
C20	-0.44334	-1.58025	5.114446
C21	-0.74559	-1.48693	3.763824
C22	-0.47873	-0.32742	3.016854
C23	0.166388	0.712888	3.697974
C24	0.490515	0.630958	5.046056
F25	0.460661	-0.59722	7.072013
F26	-0.7279	-2.70084	5.794247
F27	-1.28677	-2.55869	3.163486
F28	0.518055	1.828304	3.027365
F29	1.094982	1.658973	5.659729
C30	-4.44925	-0.99069	-3.35255
C31	-4.50627	0.050268	-2.43076
C32	-3.572	0.106969	-1.40303
C33	-2.57594	-0.86866	-1.25111
C34	-2.54596	-1.90803	-2.19321
C35	-3.46618	-1.96992	-3.23406
F36	-5.3454	-1.05691	-4.3463
F37	-5.45206	0.993272	-2.54456
F38	-3.6325	1.131491	-0.53509
F39	-1.6376	-2.88019	-2.08011
F40	-3.43144	-2.97986	-4.11335
H42	-0.18059	0.638284	-2.7222
H43	2.07861	1.745204	-0.32808
O44	2.700286	2.995312	-2.61181
O47	3.161571	0.421392	2.201211
H48	3.105254	2.208827	-2.22042
H49	2.374297	3.502718	-1.83445
H52	1.59201	0.374305	-1.51696
H54	2.519729	1.069646	2.517295
O55	1.131775	-1.91374	-0.16355
O56	-0.29656	1.955428	-0.4555
H56	0.402832	-2.48002	-0.45486
H57	-1.02434	2.053247	0.171963
H59	2.44678	-1.37527	2.549799
O60	1.93446	-2.20324	2.516036
H61	1.633212	-2.21643	1.584571
H62	2.90021	-3.25657	-2.19099
O63	2.853084	-2.30047	-2.06919

H64	2.297368	-2.17571	-1.23123
H65	0.629259	3.129303	-3.07216
O66	-0.27931	3.380289	-2.83247
H67	-0.46327	2.81386	-2.04939
H68	0.724103	3.414831	-0.28014
O69	1.22725	4.211776	-0.57808
H70	0.675727	4.458275	-1.34497
C70	0.74693	0.09132	-2.56545
O67	0.675569	-1.17407	-3.11076
H69	1.520736	-1.64801	-2.896

Table S103. $[Rh^{III\text{-}I}(NN^{F})(OH^{eq})(H_2O)_2(CH_3{}^{ax}\text{-}OH_2)]^{‡}\cdot 7H_2O$

Atom	x	y	z
Rh1	0.016144	0.125079	-0.10034
N2	-0.91119	-0.47165	1.652794
H3	4.328622	-0.03148	2.056616
C4	-1.98116	-0.98089	1.046083
O5	1.817746	1.03113	0.613573
N6	-1.85944	-0.80751	-0.27677
H7	2.438132	0.661554	-2.27251
C8	-5.16564	-3.07715	3.032239
C9	-4.53529	-3.6456	1.928447
C10	-3.50825	-2.95524	1.294005
C11	-3.08941	-1.69325	1.72945
C12	-3.74269	-1.14604	2.838893
C13	-4.7666	-1.82443	3.491588
F14	-6.14938	-3.73296	3.650062
F15	-4.90973	-4.85364	1.494224
F16	-2.90805	-3.5457	0.25045
F17	-3.40155	0.064877	3.293951
F18	-5.3771	-1.27618	4.546586
C19	0.450728	-1.06823	5.59473
C20	0.033529	-2.15962	4.839864
C21	-0.42712	-1.9651	3.542581
C22	-0.51842	-0.68775	2.965403
C23	-0.0706	0.390422	3.746377
C24	0.405548	0.208194	5.039636
F25	0.896778	-1.24457	6.84353
F26	0.097261	-3.39432	5.355189
F27	-0.75908	-3.04977	2.817601

F28	-0.10348	1.630092	3.247031
F29	0.810443	1.25932	5.763153
C30	-4.7692	-0.85268	-3.3368
C31	-5.12522	-0.43592	-2.05788
C32	-4.18475	-0.42221	-1.03311
C33	-2.85694	-0.85718	-1.22457
C34	-2.53682	-1.24685	-2.53843
C35	-3.45678	-1.24864	-3.57691
F36	-5.67189	-0.86309	-4.32472
F37	-6.37418	-0.01842	-1.8222
F38	-4.56996	0.068776	0.155336
F39	-1.2655	-1.63294	-2.82916
F40	-3.08826	-1.64172	-4.80353
O41	0.621353	0.435446	-2.22771
H42	0.091671	-0.25763	-2.65437
H43	2.443382	1.033892	-0.12822
O44	2.396814	3.601099	-1.71951
O45	3.332714	0.979148	-2.03281
O47	3.450919	-0.45784	2.172603
H48	2.877692	4.420137	-1.89063
H49	2.033172	3.661816	-0.76445
H50	3.228082	1.950689	-1.9366
H53	2.802063	0.149372	1.71109
O54	-1.4632	3.107292	-0.31016
H55	-0.63896	3.237566	0.188925
H56	-1.15756	3.088822	-1.22825
O57	0.058905	2.927203	-2.85912
H58	0.278894	1.320564	-2.53695
H59	0.908627	3.328965	-2.54273
O60	1.299226	3.457516	0.581482
H61	1.498301	2.426811	0.722489
H62	1.546238	3.920366	1.390959
H63	2.134629	-1.12102	-0.56604
C64	1.787401	-1.90102	0.084765
H65	1.44056	-1.64671	1.069296
H66	1.360768	-2.7849	-0.37365
O67	3.410865	-2.47106	0.622578
H68	3.502812	-1.73235	1.353692
H69	4.013157	-2.13602	-0.08075
O70	4.984814	-0.85383	-1.02014

H71	4.406316	-0.13636	-1.39783
H72	5.558952	-1.13447	-1.7438
O73	5.91549	0.434523	1.298705
H74	6.627925	-0.05952	1.722681
H75	5.761365	-0.01173	0.441181
H76	-0.12061	3.272936	-3.7411

Table S104. $[Rh^{III\text{-}I}(NN^{F})(OH^{eq})_2(H_2O^{ax})(CH_3{}^{ax}\text{-}OH_2)]^{-\ddagger}\cdot 8H_2O$

Atom	x	y	z
Rh1	0.087615	0.13012	-0.04886
N2	-0.94876	-0.39879	1.715823
H3	4.518518	-0.02742	1.855303
C4	-1.98147	-0.9341	1.062338
O5	1.937289	1.002638	0.648133
N6	-1.79237	-0.80255	-0.25587
H7	2.250738	0.797287	-2.17451
C8	-5.27984	-2.98755	2.917798
C9	-4.58563	-3.58159	1.868458
C10	-3.52232	-2.90788	1.27791
C11	-3.12598	-1.63277	1.699658
C12	-3.84523	-1.06108	2.755997
C13	-4.90553	-1.72425	3.365546
F14	-6.30221	-3.63105	3.496392
F15	-4.93305	-4.80705	1.447715
F16	-2.86222	-3.53485	0.292813
F17	-3.53622	0.161652	3.203012
F18	-5.58067	-1.14801	4.370285
C19	0.276077	-0.94548	5.712601
C20	-0.14291	-2.04139	4.967629
C21	-0.56796	-1.86668	3.655493
C22	-0.61887	-0.60159	3.040171
C23	-0.16755	0.482635	3.818407
C24	0.269318	0.317696	5.127374
F25	0.684236	-1.10388	6.982829
F26	-0.11243	-3.2705	5.51144
F27	-0.8952	-2.96918	2.951686
F28	-0.1586	1.714143	3.299508
F29	0.674295	1.378503	5.844123
C30	-4.57223	-1.03431	-3.42294
C31	-4.97118	-0.51215	-2.19802

C32	-4.07362	-0.44184	-1.1384
C33	-2.74708	-0.90982	-1.24092
C34	-2.37998	-1.41542	-2.50351
C35	-3.26244	-1.4793	-3.57273
F36	-5.43893	-1.11022	-4.44693
F37	-6.22538	-0.05594	-2.04817
F38	-4.50228	0.132637	-0.00188
F39	-1.12525	-1.86762	-2.70115
F40	-2.86425	-1.99227	-4.74863
O41	0.799738	0.417645	-2.00676
H42	0.41249	-0.27682	-2.5529
H43	2.457253	1.088229	-0.1695
O44	2.401244	3.75789	-1.56255
O45	3.228165	1.111501	-2.11032
O46	4.229825	-3.28623	-2.34137
O47	3.63099	-0.39739	2.046031
H48	2.656926	4.668997	-1.74308
H49	2.013041	3.751126	-0.64135
H50	3.178689	2.080506	-1.99531
H51	4.070445	-3.4594	-1.40012
H52	3.344139	-3.15417	-2.705
H53	2.950377	0.21504	1.574166
O54	-1.53911	3.123738	-0.11995
H55	-0.71315	3.163356	0.387507
H56	-1.21025	3.024773	-1.0371
O57	-0.22221	2.859622	-2.6267
H58	0.048399	1.921991	-2.46392
H59	0.586086	3.338028	-2.37564
O60	1.2789	3.434004	0.809031
H61	1.523675	2.427128	0.85321
H62	1.533886	3.815764	1.656424
H63	2.031233	-1.20611	-0.79352
C64	1.903192	-1.88984	0.030703
H65	1.629026	-1.47967	0.98589
H66	1.466305	-2.85578	-0.20617
O67	3.59262	-2.2579	0.396524
H68	3.652232	-1.58232	1.227099
H69	4.064786	-1.68338	-0.28223
O70	4.870526	-0.69913	-1.31538
H71	4.271627	0.056406	-1.64315

H72	4.923138	-1.37107	-2.01752
O73	6.220264	-0.01568	1.005818
H74	6.578412	-0.86689	1.287968
H75	5.910136	-0.18276	0.089897

Table S105. $[Rh^{III\text{-}II}(NN^{F})(OH^{ax})(H_2O^{eq})_2(CH_3{}^{ax}\text{-}OVCl_3)]^{\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.028681	-0.07128	0.032599
N2	-0.96987	-0.49342	1.855682
H3	2.094886	0.823331	1.415574
C4	-2.0252	-0.99493	1.22556
O5	1.98261	0.658421	0.438584
N6	-1.82572	-0.95521	-0.09174
H7	-0.29384	0.362889	-2.52801
C8	-5.53678	-2.57941	3.109844
C9	-4.81005	-3.36729	2.218636
C10	-3.67292	-2.8428	1.612495
C11	-3.239	-1.54057	1.881132
C12	-3.98574	-0.7712	2.778415
C13	-5.12562	-1.27745	3.392917
F14	-6.62706	-3.07089	3.692607
F15	-5.2031	-4.61389	1.956424
F16	-2.98754	-3.616	0.76548
F17	-3.61623	0.485999	3.053043
F18	-5.82951	-0.52497	4.24042
C19	-0.11545	-0.94158	5.955885
C20	-0.25594	-2.07044	5.150845
C21	-0.55056	-1.91248	3.802203
C22	-0.72151	-0.64762	3.221894
C23	-0.5884	0.464645	4.059473
C24	-0.2816	0.327674	5.407763
F25	0.169791	-1.07767	7.251633
F26	-0.10536	-3.28928	5.674674
F27	-0.6743	-3.00857	3.032404
F28	-0.77597	1.693093	3.566117
F29	-0.16082	1.409604	6.182568
C30	-4.66826	-1.23017	-3.17605
C31	-4.88655	-0.35629	-2.1135
C32	-3.95129	-0.27867	-1.08981
C33	-2.79903	-1.07534	-1.07904

C34	-2.59856	-1.93287	-2.16754
C35	-3.51747	-2.01567	-3.20725
F36	-5.55798	-1.31173	-4.16645
F37	-5.97865	0.412618	-2.09269
F38	-4.14607	0.606993	-0.09572
F39	-1.49194	-2.68983	-2.21684
F40	-3.30922	-2.84759	-4.23012
O41	0.533977	0.137685	-2.02152
H42	0.901692	-0.69407	-2.46063
H43	2.153669	1.551226	0.011826
O44	2.382467	3.173512	-0.36339
O45	-1.55156	1.188995	-3.33962
O46	1.330635	-1.94255	-3.33193
O47	2.102891	1.409934	2.989103
H48	1.785403	3.404645	-1.0989
H49	1.934915	3.549281	0.421594
H50	-1.15593	2.056301	-3.09028
H51	-1.48299	1.140977	-4.30206
H52	0.819175	-2.76023	-3.22036
H53	2.25154	-2.22807	-3.1947
H54	1.584674	2.220113	2.759331
H55	2.982282	1.716202	3.244458
O56	-0.68378	1.953778	0.126819
H57	-1.63805	1.902263	0.27957
H58	0.760852	-2.44164	1.293024
O59	0.713779	3.384824	1.79969
O60	0.177405	2.962492	-2.17527
H61	-0.2236	2.678266	-1.30184
H62	0.748563	2.203155	-2.37877
H63	0.185504	4.04927	2.25772
H64	0.076935	2.831332	1.237973
C65	1.143641	-2.24495	0.305141
H66	0.558225	-2.55912	-0.54904
H67	2.067795	-1.69843	0.178879
O68	2.128373	-3.96674	0.375581
V69	2.69268	-4.79795	-0.9111
Cl70	0.94899	-5.08488	-2.29674
Cl71	3.986181	-3.36825	-2.07035
Cl72	3.733589	-6.67457	-0.51544

Table S106. $[Rh^{III-II}(NN^{F})(OH^{eq})(H_2O)_2(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.14284	-0.05886	-0.21447
N2	-1.03887	-0.11103	1.517279
H3	3.250429	-0.42059	0.610554
C4	-2.13559	-0.53885	0.871438
O5	1.949262	0.725942	0.380759
N6	-1.84863	-0.74418	-0.40775
H7	1.923308	-0.56008	-2.16761
C8	-6.04337	-1.09665	2.58821
C9	-5.49575	-2.07059	1.756541
C10	-4.22779	-1.88115	1.216012
C11	-3.47851	-0.72724	1.478785
C12	-4.05688	0.225672	2.321892
C13	-5.31937	0.058712	2.875697
F14	-7.25489	-1.26737	3.108196
F15	-6.18262	-3.17957	1.48766
F16	-3.72861	-2.84503	0.440265
F17	-3.39527	1.363014	2.627141
F18	-5.83993	0.996958	3.667961
C19	-0.07551	-0.49687	5.607007
C20	-0.79625	-1.5045	4.970543
C21	-1.12557	-1.37647	3.625541
C22	-0.77625	-0.24048	2.874861
C23	-0.03489	0.739887	3.547509
C24	0.31593	0.629081	4.885559
F25	0.241519	-0.60856	6.896391
F26	-1.15425	-2.59417	5.646086
F27	-1.76489	-2.39109	3.024583
F28	0.372783	1.847329	2.869986
F29	1.010284	1.600587	5.482599
C30	-4.41614	-0.78253	-3.73774
C31	-4.55903	0.207945	-2.77016
C32	-3.7297	0.20195	-1.65677
C33	-2.75283	-0.78444	-1.46521
C34	-2.62391	-1.76339	-2.45994
C35	-3.44296	-1.76785	-3.58365
F36	-5.20758	-0.78635	-4.81219
F37	-5.47522	1.169781	-2.92453
F38	-3.85122	1.19883	-0.75822

F39	-1.6994	-2.72013	-2.33319
F40	-3.31026	-2.71815	-4.51173
O41	0.918744	-0.36818	-2.16401
H42	0.825011	0.442257	-2.71309
H43	1.761172	1.243654	1.176086
O44	2.919737	2.091034	-1.60996
O45	1.082038	2.025705	-3.52819
O46	3.48408	-0.62315	-2.2049
O47	3.950784	-1.07805	0.39391
H48	2.521642	1.646858	-0.78809
H49	3.442089	2.840884	-1.30122
H50	1.737555	2.251885	-2.81197
H51	1.601874	1.863726	-4.32572
H52	3.772347	-1.00704	-1.34092
H53	3.676131	0.327826	-2.11017
H54	3.901617	-1.77313	1.066136
O55	-0.5271	1.989572	-0.77758
H56	-0.01662	-2.54323	0.869136
H57	-0.69042	2.318285	-3.51624
O58	-1.61862	2.30717	-3.19698
H59	-1.08162	2.063755	-1.59448
H60	-1.00365	2.451362	-0.04306
O61	-1.6637	3.261114	1.285536
H62	-1.0279	3.037993	1.980783
H63	-2.47404	2.804021	1.548467
H64	-1.94288	3.209846	-3.3083
C65	0.647004	-2.36171	0.036685
H66	0.329519	-2.65843	-0.95107
H67	1.62923	-1.92645	0.189495
O68	1.584295	-4.11978	0.304701
V69	1.940505	-4.71822	1.786044
Cl70	0.026583	-5.10903	2.828205
Cl71	3.259098	-6.45579	1.836869
Cl72	2.843199	-3.01627	2.935441

Table S107. $[Rh^{III\text{-}II}(NN^{F})(OH^{eq})_2(H_2O^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	-0.06261	0.438012	-0.107
N2	-1.03414	-0.3575	1.586885
H3	3.763961	-1.49452	-2.10343

C4	-2.0299	-0.91253	0.901596
O5	1.54775	1.3032	0.769048
N6	-1.85322	-0.74895	-0.40653
H7	2.181408	1.456593	-1.82087
C8	-5.34144	-3.0017	2.677912
C9	-4.5531	-3.63246	1.719423
C10	-3.48541	-2.94532	1.150259
C11	-3.18131	-1.63108	1.516895
C12	-3.98837	-1.02221	2.481298
C13	-5.05998	-1.69341	3.06187
F14	-6.37019	-3.65231	3.230218
F15	-4.82196	-4.8922	1.359143
F16	-2.73964	-3.58069	0.242346
F17	-3.75119	0.237489	2.864314
F18	-5.8265	-1.08816	3.9781
C19	0.02894	-0.73366	5.640892
C20	-0.30421	-1.87015	4.911654
C21	-0.67073	-1.75112	3.57549
C22	-0.74647	-0.5039	2.932223
C23	-0.39016	0.621856	3.693039
C24	-0.00684	0.513761	5.023965
F25	0.380388	-0.83733	6.930516
F26	-0.25577	-3.07436	5.494954
F27	-0.93378	-2.8727	2.88701
F28	-0.43426	1.840609	3.13899
F29	0.30842	1.611551	5.728304
C30	-4.61376	-1.31539	-3.53333
C31	-5.00528	-0.6229	-2.39281
C32	-4.10568	-0.44487	-1.34755
C33	-2.80204	-0.96536	-1.39305
C34	-2.435	-1.65228	-2.5629
C35	-3.32119	-1.82559	-3.62001
F36	-5.47741	-1.49247	-4.54366
F37	-6.24535	-0.11642	-2.31197
F38	-4.50741	0.265823	-0.28047
F39	-1.20551	-2.16282	-2.66828
F40	-2.94876	-2.49805	-4.71656
O41	0.620623	1.063471	-1.9686
H42	0.640876	0.319153	-2.60835
H43	2.257489	1.313148	0.093279

O44	3.162036	4.189758	-0.54409
O45	3.147863	1.542124	-1.55414
O46	1.261811	-0.83406	-3.93545
O47	3.741335	-0.81311	-2.79108
H48	3.797463	4.039155	0.16713
H49	2.290626	4.146873	-0.08398
H50	3.292901	2.497305	-1.39515
H51	2.190503	-0.90391	-3.60316
H52	1.326018	-0.24981	-4.70085
H53	3.741315	0.053014	-2.32147
O54	-1.38088	2.293548	-0.0607
H56	-0.72867	2.92394	0.328027
H57	-1.44304	2.566535	-1.01787
O58	-1.10268	2.870908	-2.65342
H59	-0.39802	2.156145	-2.52255
H60	-0.60207	3.697115	-2.65586
O61	0.826088	3.682854	0.867507
H62	1.166551	2.683528	0.899889
H63	0.754215	3.956912	1.790722
H64	1.489118	-1.45839	0.538552
C64	1.287998	-1.62216	-0.51246
H65	0.461979	-2.24992	-0.81448
H66	1.764222	-1.00349	-1.25402
O67	2.658459	-2.92026	-0.68895
V68	2.774168	-4.30839	0.19776
Cl69	0.919053	-5.47971	-0.12416
Cl70	4.556648	-5.56678	-0.12203
Cl71	2.664222	-3.67431	2.32669

Table S108. $[Rh^{III\text{-}II}(NN^{F})(OH)_2(H_2O^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{-\ddagger}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.085215	-0.08115	-0.25534
N2	-1.05291	-0.35288	1.486158
H3	3.251482	-0.37728	0.444278
C4	-2.15117	-0.7476	0.835304
O5	1.889068	0.637194	0.379574
N6	-1.8931	-0.86798	-0.464
H7	1.872659	-0.24547	-2.23825
C8	-6.005	-1.4406	2.611033
C9	-5.43983	-2.39989	1.774792

C10	-4.19046	-2.16712	1.209256
C11	-3.47994	-0.98864	1.458709
C12	-4.07393	-0.04137	2.297938
C13	-5.32078	-0.25703	2.875673
F14	-7.20425	-1.65459	3.157982
F15	-6.09592	-3.53822	1.526054
F16	-3.67182	-3.11396	0.42164
F17	-3.45375	1.116421	2.553973
F18	-5.87125	0.668085	3.669796
C19	-0.12679	-0.60601	5.589101
C20	-0.82607	-1.64151	4.977275
C21	-1.14452	-1.5583	3.626582
C22	-0.80713	-0.43827	2.846447
C23	-0.08582	0.578652	3.49261
C24	0.252114	0.503742	4.83802
F25	0.182438	-0.67624	6.889535
F26	-1.17392	-2.72104	5.68557
F27	-1.76476	-2.60407	3.05623
F28	0.295913	1.66392	2.797767
F29	0.926488	1.501837	5.421482
C30	-4.5713	-0.67498	-3.70257
C31	-4.7072	0.221418	-2.64727
C32	-3.83877	0.147253	-1.56476
C33	-2.83025	-0.82634	-1.485
C34	-2.71066	-1.70651	-2.5716
C35	-3.56543	-1.63733	-3.66562
F36	-5.40518	-0.61418	-4.74876
F37	-5.66407	1.157768	-2.68501
F38	-3.97207	1.053994	-0.58041
F39	-1.75826	-2.64649	-2.56221
F40	-3.43917	-2.50222	-4.68026
O41	0.867068	-0.18893	-2.22324
H42	0.700267	0.650509	-2.71968
H43	1.695944	1.141644	1.181739
O44	2.65376	2.526406	-1.40796
O45	1.139168	2.151435	-3.51503
O46	3.515969	-0.09875	-2.35405
O47	4.033162	-0.90972	0.146593
H48	2.392543	1.824394	-0.75092
H49	2.135683	3.310255	-1.07707

H50	1.756493	2.345301	-2.73839
H51	1.712151	1.975152	-4.27131
H52	3.834262	-0.54423	-1.52928
H53	3.638216	0.846625	-2.16547
H54	4.021686	-1.74768	0.630458
O55	-0.7402	1.853256	-0.5569
H56	0.325813	-2.68474	-1.13484
H57	-1.48514	1.914397	0.057847
H58	-0.35912	3.308187	-3.21218
O59	-1.0401	3.679493	-2.62407
H60	-1.1326	2.955095	-1.96444
H61	0.281731	3.317301	-0.2543
O62	0.740464	4.157012	-0.50148
H63	0.214773	4.377029	-1.29914
C64	0.815466	-2.55944	-0.18037
H65	1.768066	-2.04621	-0.14094
H66	0.216868	-2.63935	0.715919
O67	1.528402	-4.23885	-0.09398
V68	2.14332	-5.06307	1.192425
Cl69	2.872387	-7.12041	0.861306
Cl70	3.765607	-3.77144	2.046647
Cl71	0.593837	-4.99071	2.789273

Table S109. $[Rh^{IV\text{-}II}(NN^{F})(OH^{eq})_2(H_2O^{ax})(CH_3{}^{ax}\text{-}OH_2)]^{‡}\cdot 6H_2O$

Atom	x	y	z
Rh1	0.050706	0.332741	-0.26187
N2	-0.79487	-0.32667	1.548829
H3	3.380505	0.272478	0.323164
C4	-1.84469	-0.91075	0.975128
O5	1.75412	1.254932	0.382469
N6	-1.77149	-0.79194	-0.35218
H7	2.219923	1.315048	-2.35153
C8	-4.86876	-3.06048	3.144888
C9	-4.21041	-3.66758	2.078006
C10	-3.23832	-2.95835	1.380525
C11	-2.9027	-1.64396	1.719071
C12	-3.57822	-1.05963	2.795163
C13	-4.55233	-1.75252	3.506462
F14	-5.80017	-3.7316	3.821046
F15	-4.5048	-4.92563	1.739081

F16	-2.60888	-3.57738	0.373161
F17	-3.3058	0.198389	3.158382
F18	-5.18869	-1.17038	4.525946
C19	0.686737	-0.7855	5.462527
C20	0.387694	-1.91228	4.701544
C21	-0.1162	-1.75699	3.41574
C22	-0.3625	-0.49409	2.856036
C23	-0.03318	0.62063	3.641103
C24	0.483668	0.483392	4.924564
F25	1.173167	-0.92066	6.699529
F26	0.606431	-3.13438	5.199738
F27	-0.33533	-2.86028	2.67315
F28	-0.22201	1.85443	3.154042
F29	0.776348	1.566842	5.652213
C30	-4.80089	-1.11718	-3.27013
C31	-5.10787	-0.58876	-2.0202
C32	-4.12204	-0.48198	-1.0446
C33	-2.80538	-0.92666	-1.26232
C34	-2.52974	-1.4275	-2.54508
C35	-3.49745	-1.52884	-3.53501
F36	-5.7449	-1.22209	-4.20947
F37	-6.34969	-0.16435	-1.76502
F38	-4.45415	0.093051	0.121381
F39	-1.2728	-1.82478	-2.84989
F40	-3.18527	-2.03109	-4.7344
O41	0.643512	0.705283	-2.22068
H42	0.293154	-0.00241	-2.77686
H43	2.191545	1.566921	-0.43575
O44	1.74038	4.255438	-1.53849
O45	3.068798	1.763595	-2.0946
O46	4.506235	-2.53271	-0.66913
O47	4.144533	0.004077	-0.23061
H48	2.00583	5.173399	-1.66856
H49	1.457608	4.176058	-0.59491
H50	2.843356	2.711858	-2.0529
H51	4.411362	-1.54086	-0.51621
H52	5.076927	-2.86233	0.035419
H53	4.048899	0.607392	-0.99878
O54	-1.28061	2.151486	-0.20557
H56	-0.75578	2.746264	0.373606

H57	-1.16711	2.55373	-1.12417
O58	-0.62101	3.02227	-2.58938
H59	-0.15459	2.148034	-2.65789
H60	0.108433	3.636803	-2.38242
O61	0.815751	3.56689	0.920932
H62	1.248756	2.642916	0.881589
H63	0.89546	3.88585	1.827422
H64	1.939329	-1.25688	-0.73909
C64	1.113169	-1.93682	-0.58001
H65	0.838282	-2.22967	0.422173
H66	0.418081	-2.14595	-1.3774
O67	2.181676	-3.52105	-0.84856
H68	3.149051	-3.17356	-0.74148
H69	2.089427	-3.74609	-1.78679

Rh(ONN) complexes in TFAH

Table S110. [Rh^{I}(ONN)(TFA)]$^{-}$

Atom	x	y	z
Rh1	0.205563	-0.05168	-0.07449
N2	-0.17945	-0.45918	1.759303
C3	0.69369	-0.00061	2.700169
C4	0.472547	-0.21159	4.08647
C5	-0.719	-0.92508	4.438591
C6	-1.58921	-1.36576	3.467819
C7	-1.31103	-1.12465	2.096144
C8	1.430943	0.298354	4.988551
H9	-0.93159	-1.11213	5.488578
H10	-2.49112	-1.90404	3.744156
C11	1.826385	0.713274	2.153219
C12	2.748232	1.198188	3.111481
C13	-2.09267	-1.49914	0.935161
O14	1.929593	0.866507	0.87207
N15	-1.58033	-1.12531	-0.22656
C16	0.247755	1.450555	-2.70041
O17	0.741952	0.481283	-2.03893
O18	-0.74198	2.155529	-2.49123
C19	1.086373	1.747085	-3.97847
F20	0.50095	2.665472	-4.7774
F21	2.314696	2.225239	-3.66436
F22	1.274741	0.636931	-4.73261

C23	2.534502	0.983957	4.479485
H24	3.619848	1.7438	2.762652
H25	3.26951	1.377163	5.180928
H26	1.301571	0.159507	6.058591
C27	-3.28008	-2.17195	-3.94578
C28	-2.93591	-3.17336	-3.03714
C29	-2.38878	-2.83996	-1.79787
C30	-2.18167	-1.49444	-1.45792
C31	-2.49934	-0.48907	-2.38224
C32	-3.05554	-0.8335	-3.61167
H33	-3.70029	-2.43247	-4.91403
H34	-3.08214	-4.21972	-3.29478
H35	-2.09265	-3.61718	-1.0992
H36	-2.26256	0.544511	-2.14386
H37	-3.29476	-0.0459	-4.32145
C38	-3.40859	-2.21594	1.10779
H39	-4.01466	-2.16127	0.202981
H40	-3.26628	-3.27592	1.354299
H41	-3.97161	-1.7657	1.932358

Table S111. Rh^{I}(ONN)(TFAH)

Atom	x	y	z
Rh1	-0.08512	-0.02075	-0.16872
N2	-0.32609	-0.46236	1.674301
C3	0.561603	0.097355	2.545243
C4	0.449587	-0.12967	3.939555
C5	-0.62525	-0.96859	4.364887
C6	-1.50653	-1.51285	3.454205
C7	-1.34561	-1.24212	2.07164
C8	1.400331	0.498497	4.781021
H9	-0.74713	-1.17252	5.424938
H10	-2.32088	-2.14653	3.789128
C11	1.574868	0.923035	1.950001
C12	2.480648	1.522448	2.820256
C13	-2.15843	-1.69922	0.941817
O14	1.575034	1.038081	0.625713
N15	-1.75633	-1.25697	-0.23248
C16	1.204357	1.546558	-2.39188
O17	0.316727	0.717061	-2.17423
O18	2.036694	2.088126	-1.56083
C19	1.433975	2.019579	-3.8425
F20	0.351318	1.79416	-4.59362

F21	1.72067	3.328923	-3.8862
F22	2.469493	1.340856	-4.37148
C23	2.377614	1.298851	4.212791
H24	3.265195	2.157374	2.42199
H25	3.103428	1.781002	4.862632
H26	1.35304	0.352525	5.855755
C27	-3.46695	-2.34598	-3.92993
C28	-2.98432	-3.33835	-3.07626
C29	-2.43953	-2.99884	-1.83778
C30	-2.37261	-1.6537	-1.45144
C31	-2.8339	-0.65511	-2.31883
C32	-3.39059	-1.00478	-3.54566
H33	-3.88721	-2.61375	-4.89498
H34	-3.02289	-4.38182	-3.37604
H35	-2.03818	-3.76613	-1.18271
H36	-2.73914	0.38364	-2.01949
H37	-3.75301	-0.22582	-4.21025
C38	-3.36491	-2.5662	1.178183
H39	-4.00724	-2.60696	0.298567
H40	-3.07547	-3.59244	1.435355
H41	-3.94698	-2.17404	2.01865
H42	1.935289	1.745232	-0.58115

Table S112. [Rh^{III}(ONN)$(TFA)_3$]$^-$

Atom	x	y	z
Rh1	0.579033	0.278862	-0.42151
N2	0.31215	-0.30353	1.430769
C3	1.281817	0.032569	2.29136
C4	1.187683	-0.33835	3.66602
C5	0.011214	-1.05997	4.027893
C6	-0.96562	-1.36765	3.100494
C7	-0.7965	-0.96602	1.752807
C8	2.249503	0.043049	4.508073
H9	-0.11531	-1.37198	5.061679
H10	-1.85141	-1.91881	3.397002
C11	2.375808	0.779398	1.703866
C12	3.401838	1.12656	2.605513
C13	-1.68919	-1.18052	0.599852
O14	2.348986	1.075923	0.44185
N15	-1.28099	-0.70956	-0.54082
C16	0.452486	1.66157	-3.12048
O17	1.032382	0.797646	-2.36874

O18	-0.56134	2.329043	-2.96065
C19	1.23074	1.79942	-4.46326
F20	0.699386	2.751371	-5.25505
F21	2.527172	2.118431	-4.26773
F22	1.202037	0.639735	-5.16461
C23	3.315278	0.756603	3.956345
H24	4.253717	1.686624	2.235324
H25	4.132846	1.048124	4.612799
H26	2.234203	-0.21377	5.562836
C27	-3.40904	-1.13516	-4.1406
C28	-2.73817	-2.23253	-3.59781
C29	-2.03899	-2.1071	-2.3976
C30	-2.02277	-0.86834	-1.7472
C31	-2.66813	0.246271	-2.29271
C32	-3.36917	0.099008	-3.48825
H33	-3.94582	-1.23598	-5.08049
H34	-2.74659	-3.18829	-4.11495
H35	-1.47769	-2.93229	-1.9704
H36	-2.57806	1.208159	-1.80167
H37	-3.86473	0.963323	-3.92091
C38	-2.97933	-1.92341	0.79366
H39	-3.63709	-1.80696	-0.06704
H40	-2.7662	-2.99041	0.92702
H41	-3.49335	-1.56577	1.691411
O53	-0.62379	1.876604	0.044555
C54	-0.28965	3.114766	-0.14281
O55	0.776792	3.632128	-0.40374
C56	-1.54192	4.01307	0.079812
F57	-1.30854	5.291695	-0.25565
F58	-2.61375	3.596586	-0.63309
F59	-1.91248	4.003308	1.387924
O60	1.779253	-1.36637	-0.83812
C61	1.458418	-2.59474	-0.68824
O62	0.410481	-3.12462	-0.31716
C63	2.62242	-3.54437	-1.09969
F64	2.501135	-3.88817	-2.40348
F65	3.841712	-3.00323	-0.93331
F66	2.588681	-4.68872	-0.38268

Table S113. $Rh^{III}(ONN)(TFA)_2(TFAH^{ax})$

Atom	x	y	z
Rh1	0.38624	0.122038	-0.17677

N2	0.081191	-0.26454	1.720274
C3	1.060115	0.096904	2.567882
C4	0.952501	-0.2111	3.953107
C5	-0.23847	-0.88142	4.350898
C6	-1.21904	-1.22142	3.436055
C7	-1.02772	-0.90551	2.071081
C8	2.031033	0.173441	4.78332
H9	-0.37297	-1.13612	5.398452
H10	-2.11511	-1.73989	3.756809
C11	2.173903	0.777602	1.976994
C12	3.207227	1.125096	2.835816
C13	-1.8966	-1.22558	0.916129
O14	2.143156	1.050431	0.661301
N15	-1.45763	-0.83886	-0.25099
C16	0.647888	1.490269	-2.87093
O17	0.721613	0.396622	-2.20068
O18	0.365256	2.632563	-2.51761
C19	1.01638	1.245149	-4.36189
F20	0.762667	2.323389	-5.11547
F21	2.327764	0.954352	-4.47772
F22	0.317515	0.209331	-4.87415
C23	3.117509	0.818284	4.215635
H24	4.080975	1.632437	2.440841
H25	3.947275	1.106795	4.854821
H26	2.002967	-0.04193	5.846675
C27	-3.45295	-1.17671	-3.93706
C28	-2.19265	-1.75236	-3.76006
C29	-1.53654	-1.65252	-2.53662
C30	-2.16738	-0.98896	-1.47606
C31	-3.42475	-0.39594	-1.64915
C32	-4.06401	-0.49507	-2.88364
H33	-3.94913	-1.24292	-4.90076
H34	-1.70509	-2.26407	-4.58379
H35	-0.54276	-2.06416	-2.40249
H36	-3.87355	0.166797	-0.83636
H37	-5.03252	-0.02457	-3.02455
C38	-3.15717	-2.00652	1.138696
H39	-3.61994	-2.29926	0.197728
H40	-2.91682	-2.9071	1.713706
H41	-3.88044	-1.42179	1.718524
O53	-0.67043	1.947571	0.006811
C54	-0.07861	3.036607	-0.13196

O55	1.15305	3.29956	0.129721
C56	-0.93591	4.280128	-0.4424
F57	-0.23692	5.215952	-1.07886
F58	-2.00883	3.954166	-1.16273
F59	-1.35791	4.790443	0.739207
O60	1.436318	-1.5639	-0.53623
C61	1.211296	-2.72911	-0.01968
O62	0.428207	-3.07545	0.851887
C63	2.086277	-3.79588	-0.73673
F64	2.072688	-4.95805	-0.07019
F65	1.584159	-4.01986	-1.97345
F66	3.362656	-3.40378	-0.86961
H67	1.673883	2.428728	0.349857

Table S114. $Rh^{III}(ONN)(TFA)_2(TFAH^{eq})$

Atom	x	y	z
Rh1	0.169375	0.069046	-0.27371
N2	0.008941	-0.36804	1.599767
C3	1.004947	0.088501	2.375326
C4	0.986004	-0.1616	3.778297
C5	-0.13945	-0.88906	4.260938
C6	-1.1443	-1.32016	3.414281
C7	-1.05286	-1.04426	2.030183
C8	2.069562	0.338741	4.52892
H9	-0.20714	-1.10695	5.32315
H10	-1.99309	-1.87075	3.803236
C11	2.029733	0.820601	1.680087
C12	3.077401	1.287077	2.479209
C13	-1.98171	-1.41421	0.944443
O14	1.913636	1.009947	0.380256
N15	-1.64157	-1.01764	-0.25053
C16	1.210815	1.25478	-2.89326
O17	0.402164	0.469367	-2.37973
O18	1.672308	2.350324	-2.41675
C19	1.713293	0.940635	-4.32145
F20	0.899899	1.543627	-5.21047
F21	2.957628	1.394889	-4.50579
F22	1.693875	-0.37466	-4.55273
C23	3.07375	1.037964	3.867887
H24	3.88651	1.84486	2.020373
H25	3.907302	1.420868	4.451014
H26	2.11317	0.178467	5.601129

C27	-3.85653	-1.45223	-3.79935
C28	-2.58702	-2.02344	-3.68341
C29	-1.85932	-1.89323	-2.50357
C30	-2.42557	-1.20513	-1.4221
C31	-3.69324	-0.62024	-1.53393
C32	-4.40436	-0.74786	-2.72641
H33	-4.41098	-1.54399	-4.7286
H34	-2.15215	-2.56174	-4.5202
H35	-0.86004	-2.30633	-2.41669
H36	-4.09506	-0.0438	-0.70618
H37	-5.3822	-0.28446	-2.81859
C38	-3.19681	-2.2352	1.260351
H39	-3.7163	-2.54798	0.355787
H40	-2.89169	-3.12396	1.822737
H41	-3.89406	-1.66745	1.887011
O53	-0.99239	1.731913	0.205387
C54	-0.63829	2.938011	0.010017
O55	0.305541	3.401663	-0.64543
C56	-1.57259	3.943821	0.733305
F57	-1.21989	5.210556	0.499244
F58	-2.84588	3.776423	0.325206
F59	-1.53206	3.732981	2.064551
O60	1.282672	-1.53922	-0.81048
C61	1.23205	-2.71144	-0.26501
O62	0.619402	-3.10324	0.715549
C63	2.067889	-3.71498	-1.10727
F64	2.22282	-4.88056	-0.46725
F65	1.41866	-3.96442	-2.2716
F66	3.286356	-3.23695	-1.40918
H67	1.155111	2.682805	-1.56087

Table S115. $[Rh^{III}(ONN)(TFA)_2(CH_3^{ax})]^-$

Atom	x	y	z
Rh1	0.46669	-0.0008	-0.03529
N2	0.060968	-0.33249	1.837994
C3	0.999498	0.040492	2.723536
C4	0.778788	-0.10338	4.125595
C5	-0.48659	-0.65119	4.499659
C6	-1.42619	-1.00434	3.553771
C7	-1.13256	-0.83222	2.176516
C8	1.811929	0.308916	4.98648
H9	-0.71009	-0.78213	5.555337

H10	-2.38673	-1.40807	3.856973
C11	2.200815	0.591476	2.127186
C12	3.193574	0.985876	3.051592
C13	-1.99102	-1.0917	1.014513
O14	2.292265	0.68088	0.840835
N15	-1.46324	-0.84371	-0.15448
C16	0.796914	1.19947	-2.8464
O17	1.111415	0.284492	-2.00578
O18	-0.12241	2.008138	-2.87593
C19	1.80435	1.190519	-4.03632
F20	1.545715	2.164435	-4.93133
F21	3.080136	1.35686	-3.62361
F22	1.756184	0.01264	-4.71215
C23	2.978873	0.839254	4.427615
H24	4.114572	1.416843	2.673533
H25	3.770104	1.162886	5.101628
H26	1.696203	0.225141	6.06301
C27	-3.47337	-1.25711	-3.82858
C28	-3.20416	-2.3925	-3.06312
C29	-2.55411	-2.27009	-1.83412
C30	-2.17634	-1.0022	-1.3764
C31	-2.42654	0.141062	-2.14524
C32	-3.08181	0.002107	-3.36638
H33	-3.97135	-1.35497	-4.79
H34	-3.48836	-3.37751	-3.42476
H35	-2.31526	-3.14844	-1.24085
H36	-2.07486	1.105465	-1.79305
H37	-3.26404	0.888337	-3.96726
C38	-3.4084	-1.54982	1.235013
H39	-3.97975	-1.54045	0.307804
H40	-3.43015	-2.56558	1.647693
H41	-3.89749	-0.8903	1.959853
O53	-0.75788	1.858491	0.172969
C54	-0.34102	3.065746	0.103577
O55	0.784079	3.544535	0.147634
C56	-1.54812	4.049655	-0.00357
F57	-1.17105	5.319668	-0.2488
F58	-2.42172	3.700804	-0.97904
F59	-2.25827	4.071686	1.160592
C60	1.359602	-1.84818	-0.24845
H61	1.215317	-2.15298	-1.28747
H62	2.42399	-1.72215	-0.03583

H63	0.921144	-2.5874	0.43323

Table S116. $Rh^{III}(ONN)(TFA)(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.499427	-0.03032	-0.04365
N2	0.113438	-0.29779	1.829038
C3	1.099718	0.052029	2.674551
C4	0.912066	-0.05973	4.083241
C5	-0.35761	-0.5532	4.504066
C6	-1.3407	-0.88802	3.593637
C7	-1.08397	-0.74714	2.20837
C8	1.987345	0.332519	4.905066
H9	-0.55422	-0.65859	5.567454
H10	-2.3058	-1.24714	3.932979
C11	2.295137	0.544375	2.03699
C12	3.324255	0.920458	2.910599
C13	-1.98738	-0.99377	1.07153
O14	2.342788	0.610844	0.726386
N15	-1.48309	-0.75923	-0.11035
C16	1.205228	1.300313	-2.71915
O17	1.059535	0.228453	-2.11862
O18	0.866392	2.482929	-2.34696
C19	1.895082	1.282236	-4.10091
F20	1.150867	1.942818	-5.00286
F21	3.091313	1.887418	-4.01049
F22	2.079359	0.031584	-4.53254
C23	3.149706	0.80753	4.303558
H24	4.25168	1.304966	2.499813
H25	3.974184	1.113613	4.942826
H26	1.902139	0.271282	5.985083
C27	-3.46484	-1.33184	-3.78549
C28	-3.12163	-2.43466	-3.00324
C29	-2.48961	-2.25523	-1.7725
C30	-2.19943	-0.96101	-1.32586
C31	-2.52846	0.149545	-2.11368
C32	-3.16873	-0.04301	-3.33584
H33	-3.9535	-1.47502	-4.74463
H34	-3.33848	-3.44022	-3.35176
H35	-2.19937	-3.10911	-1.16761
H36	-2.28319	1.148418	-1.76962
H37	-3.43111	0.819978	-3.94088
C38	-3.40141	-1.42644	1.330095

H39	-3.973	-1.51317	0.407315
H40	-3.4209	-2.39122	1.849382
H41	-3.88722	-0.69097	1.980905
O53	-0.22615	2.154762	-0.17995
C54	-1.19123	2.703794	0.48847
O55	-1.75247	2.276627	1.482913
C56	-1.67431	4.029716	-0.15536
F57	-0.6421	4.83363	-0.47764
F58	-2.33846	3.743574	-1.30789
F59	-2.50527	4.708504	0.639653
C60	1.229725	-1.93736	-0.16643
H61	1.161927	-2.22137	-1.2195
H62	2.271636	-1.90665	0.158992
H63	0.653855	-2.6298	0.454688
H64	0.374261	2.474894	-1.40189

Table S117. $Rh^{III}(ONN)(TFA)(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.500901	-0.14255	-0.16457
N2	0.113726	-0.24856	1.736048
C3	1.100787	0.159071	2.55373
C4	0.916251	0.153525	3.967714
C5	-0.35716	-0.29943	4.423722
C6	-1.34357	-0.6965	3.541866
C7	-1.08646	-0.6644	2.147858
C8	1.995204	0.597446	4.756634
H9	-0.5531	-0.32531	5.491815
H10	-2.30734	-1.03013	3.91018
C11	2.298609	0.597994	1.879147
C12	3.333413	1.027231	2.722488
C13	-1.98516	-1.01462	1.031706
O14	2.341837	0.581196	0.568273
N15	-1.47743	-0.88665	-0.16676
C16	1.680043	0.707798	-2.7979
O17	0.926447	-0.13126	-2.22301
O18	2.091789	1.817807	-2.41509
C19	2.140116	0.237395	-4.202
F20	2.896333	1.153055	-4.81941
F21	2.858554	-0.89825	-4.09758
F22	1.071652	-0.01868	-4.98479
C23	3.161127	1.01681	4.119469
H24	4.262572	1.373039	2.282326

H25	3.989841	1.360735	4.733429
H26	1.913347	0.615904	5.838485
C27	-3.40711	-1.80847	-3.79404
C28	-3.22915	-2.80791	-2.83749
C29	-2.61633	-2.5147	-1.61895
C30	-2.17798	-1.2101	-1.36269
C31	-2.33534	-0.20863	-2.32899
C32	-2.96107	-0.51022	-3.53487
H33	-3.87912	-2.04192	-4.74375
H34	-3.5581	-3.82278	-3.04059
H35	-2.44942	-3.29445	-0.88187
H36	-1.96148	0.788343	-2.12167
H37	-3.08669	0.268638	-4.28107
C38	-3.39854	-1.43376	1.324729
H39	-4.00508	-1.45572	0.420136
H40	-3.42202	-2.42975	1.782002
H41	-3.84833	-0.73592	2.038379
O53	-0.42068	2.043311	-0.07641
C54	0.206442	3.103708	-0.07903
O55	1.309969	3.383201	-0.67606
C56	-0.3457	4.311913	0.714286
F57	-0.64476	5.321796	-0.12146
F58	-1.45505	3.978593	1.387474
F59	0.569339	4.748103	1.596755
C60	1.242371	-2.0445	-0.14239
H61	1.16223	-2.40887	-1.16807
H62	2.286729	-1.97767	0.168754
H63	0.67427	-2.67892	0.544273
H54	1.645243	2.61197	-1.32079

Table S118. Rh^{II}(ONN)(TFA)

Atom	x	y	z
Rh1	0.468286	-0.28136	-0.18459
N2	-0.0821	-0.46791	1.684621
C3	0.800277	-0.01252	2.595822
C4	0.4844	-0.03152	3.986187
C5	-0.79548	-0.56053	4.323899
C6	-1.66843	-1.01645	3.354546
C7	-1.28866	-0.95848	1.990564
C8	1.455586	0.474178	4.873077
H9	-1.08869	-0.60026	5.369204
H10	-2.63865	-1.41256	3.633199

C11	2.034954	0.483688	2.036497
C12	2.954909	0.977775	2.972993
C13	-2.06552	-1.35315	0.801424
O14	2.217982	0.435381	0.739868
N15	-1.4764	-1.1636	-0.35095
C16	0.477137	1.224279	-2.29814
O17	1.045763	0.094508	-2.20899
O18	-0.19489	1.744031	-1.37792
C19	0.549984	1.968521	-3.64501
F20	-0.6432	1.851786	-4.27861
F21	0.789701	3.276574	-3.46138
F22	1.496261	1.474181	-4.45243
C23	2.65007	0.960974	4.347561
H24	3.903057	1.371432	2.622643
H25	3.394626	1.354101	5.035504
H26	1.268799	0.486711	5.94196
C27	-3.09514	-2.20625	-4.10034
C28	-2.80121	-3.20611	-3.17236
C29	-2.2912	-2.87378	-1.91721
C30	-2.07521	-1.52898	-1.59292
C31	-2.35622	-0.52272	-2.52526
C32	-2.87187	-0.86718	-3.77223
H33	-3.48384	-2.46992	-5.07953
H34	-2.95902	-4.25028	-3.42644
H35	-2.03473	-3.64886	-1.20073
H36	-2.15568	0.51181	-2.26872
H37	-3.08139	-0.08333	-4.49385
C38	-3.45668	-1.89617	0.974058
H39	-3.98477	-1.95336	0.022997
H40	-3.42891	-2.89933	1.415423
H41	-4.02178	-1.25499	1.657771

Table S119. [Rh^{III}(ONN)(TFA^{ax})(CH_3^{ax}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	0.338195	-0.11683	-0.17886
N2	0.027135	-0.33199	1.73206
C3	1.047124	0.045989	2.519123
C4	0.91838	-0.01904	3.937508
C5	-0.33497	-0.49573	4.422195
C6	-1.35592	-0.85857	3.563974
C7	-1.15596	-0.76068	2.165831
C8	2.029309	0.3961	4.698336

H9	-0.4901	-0.56524	5.495451
H10	-2.30691	-1.20189	3.955059
C11	2.214311	0.510636	1.814693
C12	3.281528	0.909968	2.628085
C13	-2.11055	-1.02366	1.071658
O14	2.208707	0.530517	0.499669
N15	-1.65404	-0.84622	-0.13951
C16	1.688259	-0.29407	-2.70166
O17	0.664674	0.267201	-2.23673
O18	2.369077	-1.18562	-2.13103
C19	2.176584	0.148677	-4.09677
F20	3.365487	0.763442	-3.98076
F21	2.330678	-0.92472	-4.89206
F22	1.317895	0.988831	-4.68359
C23	3.166076	0.844298	4.030732
H24	4.191633	1.275312	2.165028
H25	4.018407	1.167999	4.622787
H26	1.991553	0.372352	5.782559
C27	-3.74185	-1.52729	-3.73092
C28	-3.56995	-2.57493	-2.82568
C29	-2.90228	-2.35807	-1.62047
C30	-2.40562	-1.08184	-1.32455
C31	-2.55606	-0.03115	-2.23982
C32	-3.23564	-0.25945	-3.4332
H33	-4.25761	-1.7002	-4.67087
H34	-3.94665	-3.56664	-3.05856
H35	-2.74297	-3.17453	-0.92214
H36	-2.1374	0.943464	-2.01328
H37	-3.35822	0.556394	-4.13917
C38	-3.52596	-1.38802	1.412176
H39	-4.15524	-1.44325	0.525551
H40	-3.56794	-2.35008	1.935239
H41	-3.92779	-0.62349	2.085939
O53	-0.30008	1.83529	-0.24134
C54	-1.2309	2.375657	0.469959
O55	-1.88634	1.929645	1.40164
C56	-1.53715	3.804159	-0.06332
F57	-0.42212	4.526975	-0.25822
F58	-2.18271	3.705623	-1.25184
F59	-2.33124	4.481879	0.777344
C60	1.017204	-2.3474	-0.21688
H61	0.314158	-2.89357	-0.84826

H62	1.995089	-2.84761	-0.26415
H63	0.728525	-2.43176	0.828604
H64	1.679383	-1.50779	-1.04221

Table S120. [Rh^{III}(ONN)(TFA^{ax})(CH_3^{eq}-H-TFA^{ax})]‡

Atom	x	y	z
Rh1	0.262131	0.143214	-0.33043
N2	0.014429	-0.3476	1.572693
C3	0.998723	0.066711	2.381237
C4	0.944014	-0.2205	3.776791
C5	-0.20337	-0.94712	4.20996
C6	-1.19612	-1.33809	3.328827
C7	-1.06575	-1.01562	1.956104
C8	2.015182	0.24189	4.568495
H9	-0.29766	-1.19761	5.263099
H10	-2.05769	-1.89239	3.683466
C11	2.052888	0.805053	1.729549
C12	3.085731	1.232519	2.570505
C13	-1.97066	-1.33026	0.827698
O14	1.98338	1.040366	0.434927
N15	-1.61112	-0.88724	-0.34304
C23	3.044851	0.94401	3.950404
H24	3.915934	1.787887	2.147627
H25	3.871153	1.295746	4.563022
H26	2.031807	0.050537	5.636429
C27	-3.6254	-1.69716	-3.95029
C28	-2.90553	-2.70822	-3.31174
C29	-2.25626	-2.45929	-2.10235
C30	-2.33538	-1.18223	-1.53465
C31	-3.04573	-0.15953	-2.17341
C32	-3.69576	-0.42522	-3.37754
H33	-4.12328	-1.89639	-4.89478
H34	-2.84056	-3.69624	-3.75842
H35	-1.66876	-3.224	-1.60394
H36	-3.08055	0.828072	-1.72347
H37	-4.25126	0.366165	-3.87237
C38	-3.20545	-2.14219	1.079715
H39	-3.88679	-2.11265	0.230195
H40	-2.91594	-3.18463	1.25743
H41	-3.72525	-1.78079	1.972007
O53	-0.80957	1.904893	0.125085
C54	-0.50523	2.906745	-0.5659

O55	0.252978	2.913719	-1.57426
C56	-1.18489	4.238551	-0.19156
F57	-0.461	5.286637	-0.59299
F58	-2.38797	4.288562	-0.79954
F59	-1.37519	4.32549	1.130429
O60	1.437072	-1.50237	-0.65851
C61	1.148351	-2.7234	-0.3581
O62	0.136125	-3.21153	0.129685
C63	2.345317	-3.65268	-0.71136
F64	2.050242	-4.93769	-0.46583
F65	2.670104	-3.54457	-2.01529
F66	3.432003	-3.32959	0.017272
H67	0.504952	1.749773	-1.81821
C50	0.614548	0.51378	-2.54796
H51	1.365755	1.149353	-3.03956
H52	1.057663	-0.48064	-2.57748
H53	-0.30634	0.525752	-3.13758

Table S121. [$Rh^{III\text{-}I}$(ONN)(TFA^{eq})($TFAH^{ax}$)($CH_3{}^{ax}$-TFA)]$^{-‡}$

Atom	x	y	z
Rh1	0.881002	0.196568	-0.13349
N2	0.294743	0.168011	1.707284
C3	1.126444	0.719602	2.621295
C4	0.748237	0.819391	3.988982
C5	-0.5437	0.309824	4.322067
C6	-1.36795	-0.23401	3.358691
C7	-0.9277	-0.29864	2.013757
C8	1.67001	1.416984	4.874884
H9	-0.8814	0.364207	5.35394
H10	-2.35289	-0.60609	3.621535
C11	2.376538	1.200916	2.073843
C12	3.247528	1.787215	3.012952
C13	-1.64093	-0.81063	0.837291
O14	2.612448	1.075006	0.799652
N15	-0.99863	-0.68653	-0.29647
C16	1.057754	1.224508	-2.92753
O17	1.469967	0.310625	-2.16622
O18	0.336031	2.217451	-2.69184
C19	1.524209	1.113671	-4.40196
F20	2.308238	2.167368	-4.72491
F21	2.224919	-0.00386	-4.65308
F22	0.464653	1.127498	-5.2392

C23	2.881716	1.879624	4.366408
H24	4.201461	2.174357	2.669041
H25	3.586775	2.344836	5.053034
H26	1.428383	1.519946	5.928599
C27	-2.38562	-2.09375	-4.01818
C28	-1.75221	-2.96688	-3.13244
C29	-1.31377	-2.52019	-1.88481
C30	-1.5236	-1.18112	-1.53148
C31	-2.14973	-0.29274	-2.41359
C32	-2.58136	-0.75973	-3.6547
H33	-2.71357	-2.44716	-4.99248
H34	-1.58247	-4.00325	-3.41186
H35	-0.7874	-3.19209	-1.20997
H36	-2.27542	0.74561	-2.12256
H37	-3.06231	-0.07039	-4.3437
C38	-3.01218	-1.40808	0.979703
H39	-3.39351	-1.75528	0.019999
H40	-2.99371	-2.25251	1.677908
H41	-3.70373	-0.65849	1.381391
O42	-2.48086	2.519208	-0.60829
C43	-1.58055	3.173263	-0.11905
O44	-0.35872	3.349841	-0.54235
C45	-1.79997	3.920931	1.219461
F46	-1.37571	5.197828	1.15835
F47	-3.10074	3.935292	1.554309
F48	-1.12536	3.307281	2.214368
C49	1.905057	-2.00659	-0.06168
H50	1.786991	-1.98811	-1.13416
H51	2.788969	-1.57631	0.383897
H52	1.114067	-2.39682	0.554926
H53	-0.12404	2.804183	-1.39356
O54	2.768533	-3.74944	-0.14025
C55	1.922996	-4.70484	-0.17165
O56	0.690053	-4.68845	-0.16956
C57	2.585947	-6.1135	-0.23711
F58	3.918915	-6.09837	-0.04766
F59	2.057833	-6.93683	0.696554
F60	2.357981	-6.68173	-1.44499

Table S122. [Rh^{III-II}(ONN)(TFA^{eq})($TFAH^{ax}$)(CH_3^{ax}-$OVCl_3$)]‡

Atom	x	y	z
Rh1	0.615329	0.493898	0.676469

N2	-0.18228	0.245347	2.438135
C3	0.297798	1.049097	3.405985
C4	-0.23867	0.992893	4.723847
C5	-1.28271	0.046279	4.928043
C6	-1.74319	-0.75738	3.900401
C7	-1.16725	-0.63954	2.612466
C8	0.31756	1.869847	5.679525
H9	-1.72498	-0.04502	5.916104
H10	-2.53471	-1.47615	4.078787
C11	1.356751	1.928604	2.986562
C12	1.86174	2.776946	3.977252
C13	-1.48999	-1.39338	1.383151
O14	1.778487	1.875109	1.73754
N15	-0.78642	-1.07924	0.325777
C16	2.219588	1.614889	-1.59866
O17	1.587479	0.598242	-1.18354
O18	2.098088	2.810655	-1.2747
C19	3.289864	1.267181	-2.66266
F20	3.985967	2.340036	-3.04844
F21	4.151065	0.360669	-2.15856
F22	2.704279	0.726765	-3.74883
C23	1.339377	2.727163	5.287016
H24	2.662473	3.464669	3.727444
H25	1.765623	3.398538	6.027649
H26	-0.04765	1.868164	6.701203
C27	-0.90776	-3.0295	-3.40258
C28	-0.61714	-3.76305	-2.25191
C29	-0.603	-3.14036	-1.00385
C30	-0.87892	-1.7692	-0.91647
C31	-1.14705	-1.02368	-2.07142
C32	-1.1748	-1.66118	-3.30803
H33	-0.91243	-3.51849	-4.37222
H34	-0.38906	-4.82247	-2.32178
H35	-0.34406	-3.7013	-0.11059
H36	-1.32674	0.042611	-1.98418
H37	-1.38988	-1.0846	-4.20269
C38	-2.57435	-2.4311	1.41701
H39	-2.8638	-2.73828	0.412623
H40	-2.23646	-3.31759	1.966322
H41	-3.45177	-2.03357	1.936651
O42	-1.02387	1.990772	0.194284
C43	-0.8714	3.216429	0.098143

O44	0.17655	3.883354	-0.20499
C45	-2.0892	4.130585	0.377301
F46	-1.80673	4.967556	1.389049
F47	-2.38186	4.858442	-0.71174
F48	-3.16661	3.410564	0.710918
C49	2.291558	-1.18086	1.081763
H50	2.67211	-1.04438	0.079652
H51	2.718882	-0.60578	1.892608
H52	1.489986	-1.87688	1.269546
H53	1.020336	3.314307	-0.55923
O54	3.561289	-2.68872	1.372469
Cl55	4.432159	-5.65267	2.210585
Cl56	3.784986	-2.87382	4.455424
Cl57	1.135207	-4.25469	2.552787
V59	3.315837	-3.81889	2.529324

Table S123. $[Rh^{I-III}(ONN)(H)(CH_3)]^{‡}$

Atom	x	y	z
Rh1	0.195135	-0.07618	-0.1567
N2	-0.24057	-0.44084	1.77544
C3	0.649826	0.025015	2.665527
C4	0.440082	-0.15515	4.065033
C5	-0.75385	-0.84955	4.424773
C6	-1.64502	-1.30785	3.471322
C7	-1.36268	-1.08408	2.099994
C8	1.419293	0.360196	4.938397
H9	-0.96371	-1.02019	5.477536
H10	-2.54526	-1.83391	3.771224
C11	1.790242	0.699076	2.077542
C12	2.724459	1.18716	3.006547
C13	-2.13582	-1.49476	0.912469
O14	1.884857	0.818089	0.778634
N15	-1.62179	-1.16975	-0.25098
C23	2.522505	1.009236	4.388581
H24	3.606934	1.702661	2.641843
H25	3.278165	1.403761	5.064214
H26	1.313196	0.249638	6.012912
C27	-3.31274	-2.27835	-3.9561
C28	-2.77444	-3.25515	-3.11807
C29	-2.2369	-2.90361	-1.87939
C30	-2.23449	-1.5626	-1.47738
C31	-2.75863	-0.5784	-2.32392

C32	-3.3045	-0.94101	-3.55328
H33	-3.72628	-2.55467	-4.92147
H34	-2.76542	-4.29597	-3.42889
H35	-1.79639	-3.65628	-1.23219
H36	-2.7237	0.460969	-2.0129
H37	-3.71455	-0.1733	-4.20322
C38	-3.43514	-2.2302	1.097787
H39	-3.98597	-2.32323	0.162579
H40	-3.25671	-3.23659	1.494851
H41	-4.05956	-1.70207	1.826201
H38	0.928487	-0.91998	-1.20906
C36	0.630675	0.554543	-2.13164
H42	0.137883	0.03529	-2.95701
H43	0.176264	1.549645	-2.00552
H44	1.69316	0.681655	-2.35103

Rh(ONN^{F}) complexes in TFAH

Table S124. [Rh^{I}(ONN^{F})(TFA)]$^{-}$

Atom	x	y	z
Rh1	0.158038	0.016679	-0.01343
N2	-0.20727	-0.41235	1.820863
C3	0.659244	0.043306	2.765231
C4	0.449062	-0.19696	4.149584
C5	-0.7215	-0.95188	4.492644
C6	-1.58037	-1.40277	3.519351
C7	-1.32003	-1.12447	2.148851
C8	1.396338	0.320769	5.054136
H9	-0.92295	-1.16548	5.539573
H10	-2.46033	-1.97824	3.790745
C11	1.783138	0.776345	2.222622
C12	2.695277	1.27226	3.187713
C13	-2.09347	-1.49868	0.991123
O14	1.891263	0.929131	0.944921
N15	-1.59751	-1.06736	-0.1627
C16	0.636696	1.482599	-2.5966
O17	0.422775	0.335057	-2.06397
O18	0.771913	2.591545	-2.098
C19	0.678406	1.363354	-4.14883
F20	0.981495	2.530473	-4.74879

F21	1.586003	0.452325	-4.57314
F22	-0.52952	0.971495	-4.64183
C23	2.485293	1.038931	4.550919
H24	3.556455	1.837162	2.844321
H25	3.211487	1.439368	5.257213
H26	1.274901	0.164073	6.122441
C27	-2.95733	-2.02936	-4.03567
C28	-2.59545	-3.04764	-3.15991
C29	-2.19444	-2.73423	-1.86658
C30	-2.14967	-1.41153	-1.40527
C31	-2.51674	-0.40513	-2.31225
C32	-2.91833	-0.70541	-3.60883
F33	-3.35885	-2.32598	-5.2812
F34	-2.64007	-4.32792	-3.56632
F35	-1.8304	-3.74072	-1.05057
F36	-2.51749	0.870281	-1.92628
F37	-3.29165	0.270181	-4.44476
C38	-3.35246	-2.31324	1.1062
H39	-4.02611	-2.11064	0.269375
H40	-3.13	-3.38661	1.098911
H41	-3.8811	-2.08222	2.034587

Table S125. $Rh^{I}(ONN^{F})(TFAH)$

Atom	x	y	z
Rh1	-0.098	-0.00097	-0.15405
N2	-0.33559	-0.4486	1.68713
C3	0.565604	0.100096	2.55246
C4	0.462496	-0.13093	3.946149
C5	-0.61784	-0.95968	4.379117
C6	-1.5136	-1.49068	3.476423
C7	-1.36208	-1.21696	2.092151
C8	1.427548	0.481706	4.782989
H9	-0.73089	-1.16682	5.439622
H10	-2.33001	-2.11827	3.817353
C11	1.583167	0.914095	1.951215
C12	2.503192	1.498305	2.81634
C13	-2.18417	-1.6634	0.972361
O14	1.575342	1.032622	0.624644
N15	-1.77882	-1.21487	-0.20457
C16	1.167846	1.522136	-2.40641

O17	0.292153	0.685101	-2.16902
O18	2.001607	2.079654	-1.58711
C19	1.37081	1.998016	-3.8605
F20	0.33287	1.648403	-4.62614
F21	1.515327	3.329443	-3.91146
F22	2.483198	1.429936	-4.36292
C23	2.409781	1.271572	4.209593
H24	3.293441	2.124156	2.414483
H25	3.1477	1.742046	4.854347
H26	1.387211	0.331508	5.857413
C27	-3.31376	-2.35638	-3.9655
C28	-2.84135	-3.3312	-3.09084
C29	-2.37945	-2.96196	-1.83175
C30	-2.38116	-1.62552	-1.41142
C31	-2.85853	-0.66346	-2.31283
C32	-3.32332	-1.01928	-3.57424
F33	-3.7629	-2.70325	-5.17342
F34	-2.83177	-4.61519	-3.46258
F35	-1.90583	-3.91623	-1.01605
F36	-2.87663	0.623476	-1.95987
F37	-3.78541	-0.08581	-4.4101
C38	-3.37482	-2.55258	1.184852
H39	-4.08764	-2.46229	0.362362
H40	-3.07039	-3.60333	1.250685
H41	-3.88749	-2.29084	2.114445
H42	1.919594	1.742513	-0.60827

Table S126. [$Rh^{III}(ONN^{F})(TFA)_3$]$^-$

Atom	x	y	z
Rh1	0.664294	0.16065	-0.45519
N2	0.32801	-0.32996	1.41647
C3	1.279852	0.044225	2.280754
C4	1.151762	-0.244	3.67254
C5	-0.04663	-0.9177	4.052717
C6	-1.00851	-1.26011	3.123632
C7	-0.7992	-0.95006	1.757162
C8	2.202231	0.168402	4.513512
H9	-0.20308	-1.15994	5.100861
H10	-1.91728	-1.76262	3.435563
C11	2.393184	0.748779	1.682379

C12	3.410037	1.125953	2.579281
C13	-1.69017	-1.19305	0.616013
O14	2.38723	0.994655	0.405589
N15	-1.24937	-0.81467	-0.55318
C16	0.498502	1.235103	-3.2521
O17	1.243864	0.699725	-2.35901
O18	-0.71492	1.417627	-3.27882
C19	1.332272	1.630982	-4.50621
F20	0.668082	2.504184	-5.28819
F21	2.519049	2.183589	-4.20015
F22	1.58221	0.531092	-5.26304
C23	3.291569	0.832295	3.946716
H24	4.276659	1.653291	2.195731
H25	4.100064	1.147628	4.60314
H26	2.160142	-0.02699	5.58062
C27	-3.51375	-0.57216	-4.08693
C28	-2.37562	-1.37105	-4.03941
C29	-1.65567	-1.47772	-2.85636
C30	-2.06568	-0.80959	-1.69841
C31	-3.2136	-0.01139	-1.76979
C32	-3.93522	0.10853	-2.95006
F33	-4.21798	-0.47584	-5.22095
F34	-1.98448	-2.03757	-5.13201
F35	-0.55381	-2.22782	-2.83559
F36	-3.6388	0.649857	-0.68582
F37	-5.04294	0.860862	-2.99475
C38	-3.03005	-1.83014	0.845185
H39	-3.44141	-2.22297	-0.08549
H40	-2.93689	-2.65038	1.56197
H41	-3.73489	-1.09455	1.248154
O53	-0.54345	1.777702	-0.04756
C54	-0.31885	2.99261	-0.43455
O55	0.643141	3.502281	-0.9735
C56	-1.55635	3.869925	-0.07636
F57	-1.42432	5.129155	-0.52501
F58	-2.6981	3.369873	-0.59824
F59	-1.73115	3.940034	1.268177
O60	1.838144	-1.49843	-0.82974
C61	1.566661	-2.68752	-0.4313
O62	0.629499	-3.12485	0.228905

C63	2.682031	-3.67489	-0.88613
F64	2.880104	-3.63483	-2.21866
F65	3.859807	-3.3814	-0.28917
F66	2.377904	-4.9474	-0.56295

Table S127. $Rh^{III}(ONN^{F})(TFA)_2(TFAH^{eq})$

Atom	x	y	z
Rh1	0.299092	0.133029	-0.3396
N2	0.156586	-0.21477	1.555567
C3	1.164052	0.272333	2.295553
C4	1.17293	0.075274	3.70857
C5	0.058359	-0.6357	4.239746
C6	-0.96071	-1.09965	3.429008
C7	-0.89676	-0.87653	2.033062
C8	2.26872	0.604915	4.417066
H9	0.010642	-0.81318	5.310457
H10	-1.80229	-1.6324	3.855926
C11	2.173038	0.981618	1.554118
C12	3.237007	1.477217	2.313699
C13	-1.86319	-1.25791	0.991118
O14	2.026842	1.128499	0.252915
N15	-1.5403	-0.9216	-0.22998
C16	1.291508	1.127091	-3.03725
O17	0.474858	0.387675	-2.46805
O18	1.778946	2.236973	-2.62507
C19	1.827797	0.702007	-4.42414
F20	1.691682	1.70765	-5.30237
F21	3.129143	0.396472	-4.32055
F22	1.167266	-0.36213	-4.88568
C23	3.259379	1.280548	3.7098
H24	4.036135	2.01796	1.81869
H25	4.102892	1.686136	4.26238
H26	2.334561	0.485364	5.493336
C27	-3.98153	-1.02207	-3.65589
C28	-2.76145	-1.69596	-3.644
C29	-1.9824	-1.69598	-2.4919
C30	-2.40941	-1.037	-1.33068
C31	-3.63695	-0.36149	-1.36866
C32	-4.42268	-0.35427	-2.51553
F33	-4.73171	-1.02242	-4.75663

F34	-2.34972	-2.34221	-4.73476
F35	-0.81921	-2.34144	-2.49771
F36	-4.06486	0.30034	-0.28639
F37	-5.59264	0.288249	-2.52744
C38	-3.1204	-1.97976	1.364026
H39	-3.58523	-2.43954	0.49141
H40	-2.89501	-2.76258	2.092979
H41	-3.83891	-1.28556	1.813288
O42	-0.89813	1.807853	0.014963
C43	-0.54731	2.998867	-0.26579
O44	0.413962	3.413365	-0.92935
C45	-1.49451	4.055865	0.363169
F46	-2.7799	3.7633	0.091423
F47	-1.34265	4.059717	1.703061
F48	-1.23895	5.284822	-0.09302
O49	1.519145	-1.44211	-0.70471
C50	1.343631	-2.63525	-0.23424
O51	0.491877	-3.06153	0.529718
C52	2.452868	-3.58448	-0.77207
F53	2.251082	-4.84311	-0.35912
F54	2.481047	-3.58704	-2.11844
F55	3.664986	-3.19093	-0.33159
H56	1.271795	2.631988	-1.78838

Table S128. [$Rh^{III}(ONN^{F})(TFA)_2(CH_3^{ax})$]-

Atom	x	y	z
Rh1	0.544568	-0.09995	0.041611
N2	0.046894	-0.33506	1.913735
C3	0.972538	0.034707	2.814956
C4	0.710546	-0.04795	4.215071
C5	-0.58667	-0.52773	4.575543
C6	-1.51393	-0.874	3.617411
C7	-1.17727	-0.7675	2.241599
C8	1.736315	0.353498	5.088421
H9	-0.84406	-0.60831	5.628697
H10	-2.50098	-1.2156	3.910082
C11	2.208517	0.523492	2.238337
C12	3.195474	0.907756	3.17255
C13	-2.02202	-1.01913	1.07525
O14	2.333473	0.580708	0.951597

N15	-1.45283	-0.85961	-0.0944
C16	0.748597	0.651138	-2.87937
O17	1.346989	0.179449	-1.85164
O18	-0.44649	0.798924	-3.11794
C19	1.76958	1.001079	-4.00139
F20	1.225761	1.787197	-4.95046
F21	2.870862	1.621397	-3.54372
F22	2.183635	-0.13836	-4.62364
C23	2.939709	0.816295	4.546088
H24	4.142989	1.285883	2.803971
H25	3.725101	1.129789	5.231335
H26	1.588804	0.312136	6.163465
C27	-3.45663	-0.76954	-3.79462
C28	-2.48511	-1.73358	-3.54706
C29	-1.86192	-1.78056	-2.30821
C30	-2.20101	-0.887	-1.28801
C31	-3.19085	0.066187	-1.55534
C32	-3.81367	0.129139	-2.79605
F33	-4.06975	-0.72641	-4.98451
F34	-2.16301	-2.61758	-4.50176
F35	-0.92618	-2.71217	-2.09414
F36	-3.56885	0.927233	-0.60522
F37	-4.77258	1.035444	-3.02794
C38	-3.46437	-1.40085	1.258827
H39	-3.84917	-1.90747	0.371658
H40	-3.58391	-2.06124	2.121407
H41	-4.07048	-0.5036	1.424015
O53	-0.59347	1.820417	0.178463
C54	-0.28013	2.934923	-0.36496
O55	0.735205	3.30492	-0.93964
C56	-1.45609	3.955035	-0.22945
F57	-1.15192	5.171698	-0.7231
F58	-2.56567	3.529464	-0.88428
F59	-1.81805	4.140025	1.068164
C60	1.400225	-1.97795	-0.03277
H61	1.501083	-2.23708	-1.08721
H62	2.384398	-1.91378	0.438783
H63	0.776687	-2.71575	0.484926

Table S129. $Rh^{III}(ONN^{F})(TFA)(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.424592	-0.02966	-0.0627
N2	0.040332	-0.29378	1.823771
C3	0.938398	0.218298	2.678894
C4	0.732422	0.124235	4.088265
C5	-0.46582	-0.53501	4.495925
C6	-1.36675	-1.03357	3.575899
C7	-1.09537	-0.89936	2.18979
C8	1.716676	0.692142	4.917141
H9	-0.6732	-0.63857	5.557323
H10	-2.27384	-1.52541	3.908731
C11	2.067017	0.864519	2.049422
C12	3.008157	1.412156	2.933556
C13	-1.90587	-1.33947	1.044517
O14	2.135134	0.910075	0.741482
N15	-1.40948	-1.06058	-0.13747
C16	1.122109	1.103003	-2.79015
O17	0.739879	0.090824	-2.13095
O18	1.388883	2.255664	-2.41524
C19	1.245573	0.797899	-4.30628
F20	1.632762	1.866444	-5.0088
F21	2.131547	-0.19307	-4.52168
F22	0.048069	0.391111	-4.79029
C23	2.815357	1.313265	4.323511
H24	3.880016	1.915915	2.530252
H25	3.570405	1.752667	4.970599
H26	1.615718	0.652296	5.9967
C27	-2.71297	-2.39871	-3.91032
C28	-2.46268	-3.32509	-2.90051
C29	-2.0861	-2.87994	-1.63866
C30	-1.96295	-1.51467	-1.35078
C31	-2.21765	-0.6029	-2.38446
C32	-2.59057	-1.03486	-3.65178
F33	-3.07839	-2.81858	-5.121
F34	-2.58005	-4.63272	-3.14696
F35	-1.81149	-3.7865	-0.68679
F36	-2.11755	0.705454	-2.15353
F37	-2.84072	-0.14964	-4.61539
C38	-3.20927	-2.04839	1.264228

H39	-3.83991	-1.99476	0.375299
H40	-3.03505	-3.10528	1.493974
H41	-3.74796	-1.60165	2.103699
O42	-0.73666	2.015098	0.247956
C43	-0.26537	3.151651	0.253394
O44	0.69866	3.625074	-0.45656
C45	-0.8884	4.17483	1.231513
F46	-0.26811	5.357945	1.213217
F47	-2.18303	4.365717	0.919979
F48	-0.82837	3.682609	2.484455
C49	1.441131	-1.80068	-0.13713
H50	1.52322	-2.05601	-1.19503
H51	2.426683	-1.62306	0.297219
H52	0.908133	-2.58062	0.413805
H53	1.029754	2.947975	-1.18377

Table S130. $Rh^{II}(ONN^{F})(TFA)$

Atom	x	y	z
Rh1	0.411386	-0.22993	-0.19405
N2	-0.11627	-0.4225	1.683878
C3	0.798055	-0.03088	2.58832
C4	0.507162	-0.07275	3.986134
C5	-0.7861	-0.56346	4.335701
C6	-1.69035	-0.96507	3.372866
C7	-1.33497	-0.88436	2.001747
C8	1.512491	0.371327	4.863285
H9	-1.06118	-0.62033	5.385308
H10	-2.66563	-1.34002	3.662108
C11	2.047309	0.42039	2.017537
C12	3.002027	0.858862	2.949087
C13	-2.13032	-1.25904	0.826351
O14	2.210571	0.382179	0.721217
N15	-1.56361	-1.03679	-0.33731
C16	0.523126	1.310943	-2.26993
O17	0.882189	0.087969	-2.24155
O18	0.102937	1.931741	-1.27409
C19	0.547547	1.991268	-3.65187
F20	-0.43598	1.467178	-4.4211
F21	0.34514	3.310747	-3.56221
F22	1.716807	1.781919	-4.27863

C23	2.718276	0.82288	4.325608
H24	3.9603	1.219324	2.591295
H25	3.489221	1.168521	5.009939
H26	1.347847	0.36559	5.935773
C27	-2.96348	-2.30836	-4.10397
C28	-2.6771	-3.25041	-3.1182
C29	-2.26892	-2.82416	-1.85931
C30	-2.14148	-1.46424	-1.55385
C31	-2.44073	-0.53688	-2.55934
C32	-2.84861	-0.94823	-3.82358
F33	-3.36185	-2.70938	-5.31103
F34	-2.79704	-4.55389	-3.38357
F35	-1.9794	-3.74078	-0.92217
F36	-2.35471	0.768625	-2.30266
F37	-3.14351	-0.04736	-4.75986
C38	-3.48962	-1.87275	0.991962
H39	-4.08763	-1.75493	0.086788
H40	-3.3954	-2.94513	1.198332
H41	-4.0229	-1.41267	1.827124

Table S131. $[Rh^{III}(ONN^{F})(TFA^{ax})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.343324	-0.02003	-0.17263
N2	-0.00978	-0.26966	1.726048
C3	0.996589	0.08373	2.538716
C4	0.835986	0.006857	3.955028
C5	-0.43397	-0.45823	4.407956
C6	-1.4402	-0.79762	3.524242
C7	-1.20896	-0.68693	2.131153
C8	1.933791	0.400965	4.741901
H9	-0.61321	-0.5376	5.476561
H10	-2.40226	-1.1367	3.890776
C11	2.186961	0.538003	1.862996
C12	3.239922	0.918979	2.704554
C13	-2.13283	-0.95567	1.018612
O14	2.213991	0.55998	0.549879
N15	-1.65257	-0.7517	-0.18165
C16	1.456077	-0.29875	-2.83076
O17	0.623393	0.419074	-2.22643
O18	2.04295	-1.30969	-2.36012

C19	1.727158	0.049952	-4.31
F20	2.911725	-0.4215	-4.71295
F21	0.763813	-0.51957	-5.06673
F22	1.697157	1.370285	-4.51161
C23	3.09105	0.841946	4.102532
H24	4.164471	1.277779	2.265902
H25	3.933249	1.150074	4.716757
H26	1.872897	0.368853	5.824651
C27	-3.49033	-1.81409	-3.82053
C28	-3.24168	-2.79112	-2.85875
C29	-2.67291	-2.42421	-1.64531
C30	-2.34962	-1.09181	-1.35793
C31	-2.60228	-0.12678	-2.34185
C32	-3.17208	-0.48235	-3.56146
F33	-4.03918	-2.15411	-4.98573
F34	-3.54742	-4.06758	-3.10361
F35	-2.41781	-3.37603	-0.73167
F36	-2.31075	1.149548	-2.11532
F37	-3.42234	0.449217	-4.48077
C38	-3.52861	-1.41562	1.30607
H39	-4.16256	-1.34902	0.421991
H40	-3.52666	-2.45358	1.656924
H41	-3.96039	-0.78842	2.0911
O53	-0.15258	1.971278	-0.07375
C54	-1.20615	2.46702	0.4815
O55	-2.11458	1.922622	1.095385
C56	-1.22106	4.014328	0.309292
F57	-0.18474	4.571245	0.970138
F58	-1.12494	4.366138	-0.98606
F59	-2.35257	4.543706	0.798495
C60	1.060817	-2.23091	-0.08817
H61	0.079119	-2.6976	-0.01269
H62	1.676606	-2.95009	-0.64956
H63	1.541831	-2.15122	0.885499
H64	1.513952	-1.54398	-1.20302

Table S132. [$Rh^{III}(ONN^{F})(TFA^{ax})(CH_3{}^{eq}$-H-$TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.225999	0.175784	-0.34274
N2	-0.0014	-0.33517	1.555767

C3	0.981527	0.090117	2.356574
C4	0.928261	-0.17044	3.758526
C5	-0.22291	-0.88019	4.208404
C6	-1.2177	-1.28084	3.335818
C7	-1.0856	-0.98917	1.956032
C8	2.001615	0.302962	4.538021
H9	-0.31878	-1.10772	5.266416
H10	-2.08196	-1.82156	3.703852
C11	2.034957	0.818221	1.693382
C12	3.071128	1.258773	2.52204
C13	-1.98641	-1.33998	0.843796
O14	1.960761	1.033277	0.394395
N15	-1.64203	-0.90085	-0.34117
C23	3.03267	0.992021	3.905965
H24	3.899605	1.807881	2.088157
H25	3.860507	1.352057	4.511406
H26	2.01934	0.132268	5.609352
C27	-3.496	-1.86534	-4.00522
C28	-3.0029	-2.88533	-3.1955
C29	-2.42602	-2.57561	-1.96731
C30	-2.33513	-1.25096	-1.51742
C31	-2.83287	-0.24371	-2.35436
C32	-3.41172	-0.53983	-3.58302
F26	-4.05292	-2.1567	-5.18
F27	-3.08568	-4.15487	-3.59727
F28	-1.94747	-3.56984	-1.21334
F29	-2.75449	1.034651	-1.9696
F30	-3.889	0.437983	-4.35526
C38	-3.20252	-2.17288	1.108705
H39	-3.94267	-2.0672	0.314205
H40	-2.907	-3.22649	1.16828
H41	-3.66263	-1.89156	2.058802
O53	-0.80434	1.924706	0.239489
C54	-0.57281	2.944614	-0.45434
O55	0.100413	2.983051	-1.5189
C56	-1.14135	4.291452	0.038054
F57	-0.13321	5.064091	0.474908
F58	-1.76356	4.927029	-0.9652
F59	-2.01159	4.119972	1.039584
O60	1.325421	-1.48122	-0.83163

C61	1.200782	-2.65528	-0.30035
O62	0.428891	-3.06495	0.552832
C63	2.249793	-3.62601	-0.91552
F64	2.095187	-4.86962	-0.44107
F65	2.128197	-3.67682	-2.25863
F66	3.50248	-3.22304	-0.62734
H67	0.372057	1.815886	-1.79581
C50	0.556304	0.645211	-2.56725
H51	1.391297	1.229644	-2.97722
H52	0.89218	-0.38821	-2.63427
H53	-0.32466	0.781137	-3.20175

Table S133. $[Rh^{III\text{-}I}(ONN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-\ddagger}$

Atom	x	y	z
Rh1	0.519061	-0.03355	-0.23235
N2	0.10479	-0.20885	1.645249
C3	0.980421	0.340723	2.515833
C4	0.744894	0.301871	3.919826
C5	-0.45958	-0.34511	4.336591
C6	-1.33104	-0.88945	3.419809
C7	-1.03479	-0.8134	2.033806
C8	1.710526	0.895563	4.754259
H9	-0.6851	-0.40523	5.398103
H10	-2.23933	-1.38076	3.751951
C11	2.134688	0.951595	1.892409
C12	3.061499	1.52456	2.785938
C13	-1.8139	-1.31748	0.909023
O14	2.24824	0.932731	0.596557
N15	-1.30173	-1.06583	-0.27814
C16	0.850856	1.261102	-2.91213
O17	0.85987	0.148571	-2.30694
O18	0.735732	2.419735	-2.48326
C19	0.972076	1.089223	-4.44987
F20	1.063794	2.262715	-5.09492
F21	2.052288	0.353935	-4.78266
F22	-0.11959	0.444644	-4.9345
C23	2.832235	1.484825	4.169247
H24	3.948964	2.001488	2.382952
H25	3.573942	1.942175	4.821295
H26	1.578471	0.893335	5.831988

C27	-2.64808	-2.5513	-3.98359
C28	-2.3272	-3.44071	-2.96259
C29	-1.9268	-2.95179	-1.72355
C30	-1.8478	-1.57582	-1.47045
C31	-2.17072	-0.70142	-2.51798
C32	-2.57062	-1.17927	-3.7607
F33	-3.04387	-3.01616	-5.17513
F34	-2.41029	-4.76035	-3.17625
F35	-1.60134	-3.82499	-0.7605
F36	-2.11686	0.615359	-2.32412
F37	-2.89795	-0.329	-4.73857
C38	-3.09633	-2.06676	1.130755
H39	-3.73161	-2.02735	0.243396
H40	-2.88908	-3.11947	1.353176
H41	-3.64923	-1.64118	1.971973
O42	-1.60832	2.70707	0.185807
C43	-0.66341	3.418797	0.45287
O44	0.444408	3.61019	-0.2191
C45	-0.63795	4.234731	1.769868
F46	-0.25029	5.510239	1.568976
F47	-1.85319	4.261285	2.340983
F48	0.21963	3.677461	2.649614
C49	1.754334	-2.10718	-0.25871
H50	1.697381	-2.07151	-1.33631
H51	2.57651	-1.61232	0.2343
H52	1.017887	-2.64459	0.316192
H53	0.505942	3.0318	-1.05856
O54	2.844522	-3.75736	-0.39628
C55	2.371719	-4.71697	0.304525
O56	1.363595	-4.77976	1.006971
C57	3.271761	-5.98693	0.195308
F58	4.546638	-5.72748	0.567471
F59	2.828935	-6.99557	0.971171
F60	3.313792	-6.45053	-1.07634

Table S134. [$Rh^{III-II}(ONN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Atom	x	y	z
Rh1	0.670719	0.596704	0.885172
N2	-0.26102	0.453822	2.594094
C3	0.193186	1.256437	3.571156

C4	-0.43243	1.259102	4.853685
C5	-1.5454	0.38041	5.001467
C6	-1.98535	-0.41364	3.95983
C7	-1.31179	-0.36517	2.713165
C8	0.10924	2.119433	5.827571
H9	-2.05808	0.338118	5.958284
H10	-2.83286	-1.07554	4.096143
C11	1.3219	2.074828	3.203976
C12	1.810433	2.908537	4.215597
C13	-1.5976	-1.12625	1.484068
O14	1.811251	1.989949	1.983159
N15	-0.78984	-0.89386	0.476471
C16	2.077333	1.437387	-1.67052
O17	1.680346	0.478592	-0.94215
O18	1.961426	2.662407	-1.50609
C19	2.787977	0.944963	-2.95759
F20	3.232807	1.956621	-3.70638
F21	3.829921	0.152896	-2.64827
F22	1.920569	0.21955	-3.70018
C23	1.203706	2.910219	5.487626
H24	2.660269	3.549853	4.007992
H25	1.6192	3.570501	6.244337
H26	-0.32158	2.162137	6.822335
C27	-0.50212	-2.98011	-3.16984
C28	-0.47214	-3.68789	-1.9702
C29	-0.62487	-3.0067	-0.76793
C30	-0.81667	-1.61853	-0.73271
C31	-0.84046	-0.93036	-1.95379
C32	-0.68771	-1.59855	-3.16204
F33	-0.36142	-3.62573	-4.32556
F34	-0.2908	-5.00854	-1.97741
F35	-0.55476	-3.69439	0.380164
F36	-1.02779	0.39039	-1.96536
F37	-0.72707	-0.92527	-4.31088
C38	-2.75042	-2.08383	1.439901
H39	-3.05132	-2.28675	0.410729
H40	-2.47382	-3.0356	1.906526
H41	-3.60589	-1.67247	1.981441
O42	-0.85889	2.253782	0.456425
C43	-0.60733	3.460171	0.357858

O44	0.432247	4.029773	-0.13014
C45	-1.64469	4.448002	0.941191
F46	-1.45694	4.521068	2.275362
F47	-1.52632	5.674838	0.42798
F48	-2.89	4.005045	0.717136
C49	2.370212	-0.94922	1.599867
H50	2.48077	-1.22395	0.55937
H51	2.956692	-0.13358	1.999215
H52	1.656584	-1.45534	2.234247
H53	1.105698	3.363217	-0.59878
O54	3.769443	-2.24315	2.12803
Cl55	5.011562	-5.10264	2.79094
Cl56	1.613067	-4.08701	3.336005
Cl57	2.887297	-4.29427	0.005381
V59	3.404553	-3.8384	2.084422

Rh(ONN^{NMe_2}) complexes in TFAH

Table S135. [Rh^{I}(ONN^{NMe_2})(TFA)]$^{-}$

Atom	x	y	z
Rh1	0.198924	-0.02099	-0.07458
N2	-0.18037	-0.37981	1.77369
C3	0.670565	0.132865	2.707903
C4	0.464936	-0.05625	4.09857
C5	-0.73668	-0.76675	4.486351
C6	-1.56965	-1.27251	3.504574
C7	-1.27621	-1.08398	2.129069
C8	1.45336	0.444807	4.975089
H10	-2.47239	-1.80702	3.776924
C11	1.792475	0.849125	2.136354
C12	2.729366	1.348312	3.071827
C13	-2.03646	-1.53331	0.980007
O14	1.8826	0.985046	0.852702
N15	-1.53772	-1.1735	-0.19285
C16	0.196828	1.389409	-2.7555
O17	0.725505	0.465477	-2.0569
O18	-0.8239	2.058338	-2.57976
C19	1.03271	1.675405	-4.03811
F20	0.427851	2.558886	-4.86159

F21	2.248319	2.190927	-3.73404
F22	1.249889	0.551346	-4.76396
C23	2.548761	1.126798	4.44091
H24	3.594453	1.88983	2.700592
H25	3.307129	1.502522	5.127026
H26	1.381322	0.262311	6.040822
C27	-3.16856	-2.42379	-3.87968
C28	-2.78969	-3.37652	-2.9333
C29	-2.26467	-2.97608	-1.70447
C30	-2.11522	-1.61159	-1.41265
C31	-2.46645	-0.65432	-2.37537
C32	-3.00018	-1.06595	-3.594
H33	-3.57182	-2.73649	-4.83969
H34	-2.89144	-4.43672	-3.15311
H35	-1.94106	-3.71434	-0.97635
H36	-2.272	0.396049	-2.17438
H37	-3.26603	-0.31525	-4.33371
C38	-3.32053	-2.29998	1.174777
H39	-3.91549	-2.32272	0.261396
H40	-3.13377	-3.33704	1.481981
H41	-3.91634	-1.83208	1.966303
N42	-1.00515	-0.93412	5.876661
C43	-1.37113	0.298313	6.576485
H44	-0.70162	1.106924	6.281984
H45	-2.40866	0.610986	6.356834
H46	-1.28273	0.148417	7.659639
C46	-1.87874	-2.03268	6.243812
H47	-2.94408	-1.86424	5.992641
H48	-1.55165	-2.95028	5.747295
H49	-1.82168	-2.18548	7.328122

Table S136. $Rh^{I}(ONN^{NMe_2})(TFAH)$

Atom	x	y	z
Rh1	-0.26258	0.203985	-0.15186
N2	-0.48397	-0.20573	1.705292
C3	0.38789	0.392863	2.568035
C4	0.378186	0.089982	3.95092
C5	-0.64574	-0.82552	4.416703
C6	-1.47781	-1.43568	3.482526
C7	-1.37236	-1.12157	2.108468

C8	1.409859	0.657584	4.740254
H10	-2.23317	-2.14205	3.802366
C11	1.340357	1.274825	1.948832
C12	2.314092	1.826973	2.775542
C13	-2.13516	-1.67647	0.985226
O14	1.222162	1.502643	0.642252
N15	-1.77759	-1.21339	-0.19574
C16	1.327214	1.301288	-2.44466
O17	0.287528	0.683359	-2.19849
O18	2.179342	1.822608	-1.61993
C19	1.693864	1.557885	-3.92176
F20	1.163297	0.618715	-4.71261
F21	1.203471	2.756013	-4.29762
F22	3.021996	1.570548	-4.10376
C23	2.339053	1.497879	4.146904
H24	3.060666	2.491156	2.351765
H25	3.133735	1.914511	4.760733
H26	1.500473	0.395375	5.786997
C27	-3.38423	-2.4975	-3.87738
C28	-2.80172	-3.42987	-3.01849
C29	-2.28892	-3.02803	-1.78479
C30	-2.3559	-1.68032	-1.4086
C31	-2.91727	-0.73951	-2.28152
C32	-3.44045	-1.15229	-3.50336
H33	-3.77924	-2.81343	-4.83856
H34	-2.7369	-4.47432	-3.3104
H35	-1.81018	-3.74587	-1.12562
H36	-2.92407	0.305916	-1.98952
H37	-3.88097	-0.41844	-4.17223
C38	-3.2446	-2.661	1.234722
H39	-3.8727	-2.78927	0.353238
H40	-2.84938	-3.64479	1.516374
H41	-3.87097	-2.31442	2.063604
H42	1.90977	1.718545	-0.61567
N43	-0.72916	-1.11595	5.790639
C44	-1.41895	-2.3359	6.17936
H45	-1.19548	-2.54386	7.230394
H46	-2.51725	-2.2724	6.079767
H47	-1.0615	-3.17736	5.580463
C47	-1.05554	0.000551	6.684962

H48	-0.70671	-0.22521	7.69842
H49	-0.57436	0.9172	6.347614
H50	-2.14311	0.179134	6.726921

Table S137. [$Rh^{III}(ONN^{NMe_2})(TFA)_3$]$^-$

Atom	x	y	z
Rh1	0.593303	0.280273	-0.42736
N2	0.345287	-0.26179	1.438618
C3	1.305259	0.114832	2.298955
C4	1.201336	-0.17588	3.68763
C5	0.034096	-0.93013	4.092091
C6	-0.94067	-1.24876	3.14858
C7	-0.76689	-0.89166	1.794204
C8	2.215393	0.339776	4.521364
H9	-1.81926	-1.81039	3.438268
C10	2.377387	0.872318	1.684584
C11	3.371451	1.327606	2.572549
C12	-1.66555	-1.15489	0.654883
O13	2.359048	1.099014	0.406457
N14	-1.26577	-0.72513	-0.50492
C15	0.438248	1.637058	-3.14724
O16	1.019726	0.778315	-2.39225
O17	-0.57426	2.308531	-2.98965
C18	1.207445	1.762846	-4.49665
F19	0.679423	2.717083	-5.28833
F20	2.508588	2.069309	-4.31358
F21	1.161648	0.600682	-5.19378
C22	3.260099	1.065991	3.943756
H23	4.198628	1.907516	2.177473
H24	4.028752	1.467126	4.601706
H25	2.159053	0.223002	5.596624
C26	-3.37578	-1.34797	-4.08619
C27	-2.74616	-2.4236	-3.45718
C28	-2.05276	-2.23233	-2.26194
C29	-2.00192	-0.9498	-1.70292
C30	-2.60569	0.141633	-2.33666
C31	-3.29976	-0.0708	-3.52607
H32	-3.90764	-1.50053	-5.0219
H33	-2.78102	-3.41429	-3.9029
H34	-1.51706	-3.04072	-1.77346

H35	-2.48775	1.134085	-1.91713
H36	-3.76207	0.775149	-4.02653
C37	-2.95301	-1.89281	0.8855
H38	-3.6176	-1.80968	0.026218
H39	-2.74069	-2.95423	1.059375
H40	-3.45993	-1.49946	1.772292
O41	-0.61588	1.877954	0.020488
C42	-0.29547	3.115508	-0.19234
O43	0.768434	3.642026	-0.44653
C44	-1.5635	4.001703	-0.01478
F45	-1.34542	5.271699	-0.39201
F46	-2.62144	3.544474	-0.72217
F47	-1.94736	4.032491	1.289678
O48	1.787726	-1.36416	-0.8567
C49	1.4769	-2.58851	-0.66898
O50	0.459447	-3.11322	-0.21333
C51	2.607564	-3.56456	-1.10735
F52	3.723715	-2.9633	-1.54522
F53	2.95868	-4.36374	-0.07103
F54	2.16423	-4.37298	-2.0987
N55	-0.10981	-1.28402	5.449662
C56	-1.44427	-1.61562	5.918508
H57	-1.4382	-1.62475	7.013766
H58	-2.15792	-0.85749	5.585592
H59	-1.80012	-2.6062	5.580922
C60	0.900509	-2.1951	5.99447
H61	0.672315	-3.24664	5.749708
H62	1.883697	-1.95798	5.590666
H63	0.935498	-2.09719	7.085658

Table S138. $Rh^{III}(ONN^{NMe_2})(TFA)_2(TFAH^{ax})$

Atom	x	y	z
Rh1	0.370226	0.1511	-0.17197
N2	0.095118	-0.23306	1.730955
C3	1.095069	0.09711	2.574946
C4	1.052225	-0.28067	3.942539
C5	-0.15356	-0.9558	4.39023
C6	-1.13117	-1.29562	3.438582
C7	-0.96905	-0.93658	2.092627
C8	2.225144	-0.03006	4.698262

N9	-0.30649	-1.31736	5.716472
H10	-2.02751	-1.81886	3.74101
C11	2.203203	0.763054	1.955334
C12	3.310701	1.013554	2.751803
C13	-1.86296	-1.25347	0.952184
O14	2.118458	1.093791	0.652463
N15	-1.46507	-0.83364	-0.21732
C16	0.647557	1.494126	-2.87665
O17	0.675675	0.397016	-2.20993
O18	0.430054	2.648233	-2.51549
C19	0.972862	1.234675	-4.3754
F20	2.255452	0.844138	-4.51927
F21	0.187127	0.259231	-4.88273
F22	0.789881	2.334352	-5.11901
C23	3.306674	0.599402	4.101238
H24	4.181187	1.495726	2.319556
H25	4.202966	0.766451	4.692163
H26	2.305477	-0.36959	5.722521
C27	-3.56962	-1.1576	-3.84441
C28	-2.29235	-1.70829	-3.7163
C29	-1.59945	-1.61178	-2.51295
C30	-2.20841	-0.97667	-1.423
C31	-3.48218	-0.40725	-1.54788
C32	-4.15957	-0.50307	-2.76213
H33	-4.09583	-1.22176	-4.79233
H34	-1.82095	-2.19752	-4.56278
H35	-0.59308	-2.00245	-2.41695
H36	-3.91577	0.134069	-0.71254
H37	-5.14182	-0.05146	-2.86481
C38	-3.09551	-2.07322	1.189628
H39	-3.583	-2.34808	0.25586
H40	-2.80809	-2.98504	1.723921
H41	-3.81259	-1.52859	1.814313
O42	-0.70843	1.966496	-0.02274
C43	-0.11955	3.059851	-0.13354
O44	1.099137	3.330372	0.172219
C45	-0.97244	4.297032	-0.48036
F46	-0.25561	5.236272	-1.09238
F47	-2.01474	3.963151	-1.24168
F48	-1.44463	4.809927	0.681622

O49	1.460405	-1.51916	-0.49546
C50	1.21299	-2.70431	-0.04263
O51	0.367951	-3.09816	0.748881
C52	2.15978	-3.7337	-0.72266
F53	2.121566	-4.91591	-0.09073
F54	1.755559	-3.93166	-1.99823
F55	3.435503	-3.31613	-0.74899
H56	1.625971	2.456507	0.388601
C57	-1.29178	-2.32888	6.070739
H58	-1.05939	-2.70293	7.071872
H59	-2.32204	-1.93779	6.087737
H60	-1.24057	-3.16961	5.375054
C61	-0.06018	-0.35791	6.796878
H62	-1.01562	-0.02425	7.227031
H63	0.532684	-0.81585	7.596998
H64	0.463731	0.520154	6.426067

Table S139. $Rh^{III}(ONN^{NMe2})(TFA)_2(TFAH^{eq})$

Atom	x	y	z
Rh1	0.161821	0.096762	-0.25676
N2	-0.02524	-0.33352	1.614964
C3	0.965816	0.099176	2.418716
C4	0.952992	-0.18636	3.809983
C5	-0.2188	-0.88164	4.312567
C6	-1.19387	-1.31805	3.401534
C7	-1.0713	-1.03588	2.031019
C8	2.110739	0.185394	4.530544
N9	-0.3426	-1.15886	5.666425
H10	-2.07056	-1.84515	3.752369
C11	2.017935	0.793408	1.724516
C12	3.117467	1.166535	2.501466
C13	-1.98961	-1.41015	0.93377
O14	1.894788	1.023903	0.429574
N15	-1.64833	-0.99903	-0.25488
C16	1.197252	1.24666	-2.90748
O17	0.398273	0.467404	-2.37446
O18	1.680233	2.339554	-2.44241
C19	1.687578	0.93438	-4.33988
F20	1.167999	1.834028	-5.19544
F21	3.024165	1.010679	-4.39998

F22	1.307049	-0.28578	-4.72461
C23	3.145376	0.839913	3.869386
H24	3.949756	1.680603	2.032535
H25	4.033234	1.105104	4.437561
H26	2.222475	-0.07545	5.574468
C27	-3.8318	-1.49081	-3.81726
C28	-2.5578	-2.04836	-3.6849
C29	-1.84007	-1.89769	-2.50169
C30	-2.41921	-1.20249	-1.43232
C31	-3.69099	-0.63057	-1.56051
C32	-4.39322	-0.77844	-2.75662
H33	-4.37907	-1.59956	-4.74914
H34	-2.11205	-2.59259	-4.51206
H35	-0.83837	-2.30086	-2.40337
H36	-4.10468	-0.04963	-0.74151
H37	-5.37503	-0.32551	-2.86085
C38	-3.18992	-2.25913	1.232961
H39	-3.70267	-2.56593	0.322594
H40	-2.86489	-3.15119	1.779101
H41	-3.89793	-1.71655	1.869968
O42	-0.99187	1.77419	0.187495
C43	-0.61394	2.972356	-0.01639
O44	0.343575	3.415623	-0.66481
C45	-1.54089	4.001861	0.682653
F46	-1.16065	5.259655	0.442909
F47	-2.8103	3.855913	0.253812
F48	-1.52849	3.804113	2.016827
O49	1.288534	-1.51599	-0.75913
C50	1.205192	-2.69907	-0.24577
O51	0.537933	-3.11728	0.688697
C52	2.081677	-3.68629	-1.06562
F53	2.227978	-4.8564	-0.43009
F54	1.474378	-3.93385	-2.25336
F55	3.304903	-3.19481	-1.32398
H56	1.178369	2.680282	-1.58038
C57	-1.2788	-2.18734	6.094748
H58	-1.03133	-2.47536	7.120705
H59	-2.32875	-1.84921	6.085427
H60	-1.18474	-3.07294	5.461605
C61	-0.18514	-0.09026	6.657916

H62	-1.1707	0.266358	6.993766
H63	0.362181	-0.45733	7.533394
H64	0.35143	0.755686	6.234786

Table S140. [$Rh^{III}(ONN^{HNMe_2})(TFA)_2(TFAH^{eq})]^+$

Atom	x	y	z
Rh1	0.554095	0.267005	-0.48031
N2	0.360668	-0.3338	1.37706
C3	1.334266	0.010933	2.218587
C4	1.266557	-0.33702	3.605348
C5	0.087991	-1.06839	3.945393
C6	-0.91645	-1.37888	3.052063
C7	-0.7579	-0.98351	1.708996
C8	2.329281	0.062318	4.429058
H9	-1.801	-1.92885	3.348971
C10	2.428322	0.761009	1.610762
C11	3.474278	1.117105	2.503609
C12	-1.65955	-1.21933	0.568783
O13	2.383998	1.045999	0.366176
N14	-1.26266	-0.74482	-0.57476
C15	0.369402	1.810835	-3.0643
O16	0.923398	0.854215	-2.39836
O17	-0.59684	2.513014	-2.80639
C18	1.116637	2.008989	-4.41544
F19	0.58231	3.013685	-5.12835
F20	2.420086	2.28964	-4.22214
F21	1.045276	0.890905	-5.17279
C22	3.402074	0.767617	3.84666
H23	4.318648	1.674818	2.114761
H24	4.220615	1.06821	4.495768
H25	2.348936	-0.12676	5.500424
C26	-3.29675	-1.31205	-4.20347
C27	-2.71198	-2.40514	-3.56093
C28	-2.04848	-2.23184	-2.34707
C29	-1.9801	-0.94967	-1.78929
C30	-2.53936	0.15902	-2.43319
C31	-3.20772	-0.03687	-3.63977
H32	-3.8058	-1.45056	-5.15312
H33	-2.75862	-3.39302	-4.00994
H34	-1.55075	-3.05911	-1.84966

H35	-2.41161	1.148773	-2.00831
H36	-3.64041	0.818614	-4.14953
C37	-2.93835	-1.97694	0.775782
H38	-3.6083	-1.85506	-0.07457
H39	-2.72352	-3.04538	0.894105
H40	-3.44812	-1.62651	1.679481
O41	-0.67888	1.807237	0.078766
C42	-0.32137	3.056928	0.038103
O43	0.774123	3.562068	-0.08781
C44	-1.57367	3.94929	0.268064
F45	-1.31004	5.242609	0.052282
F46	-2.61012	3.596413	-0.51708
F47	-1.99234	3.828379	1.559169
O48	1.710928	-1.35084	-1.06134
C49	1.481599	-2.5582	-0.70251
O50	0.609529	-3.02384	0.033812
C51	2.482092	-3.57443	-1.32179
F52	1.819	-4.42214	-2.1385
F53	3.470671	-3.01034	-2.02491
F54	3.04456	-4.31598	-0.33985
N55	-0.02173	-1.4656	5.377981
C56	-0.62936	-0.36266	6.214718
H57	-0.07291	0.553589	6.020146
H58	-1.66845	-0.24209	5.909006
H59	-0.56653	-0.63898	7.268978
C60	-0.68489	-2.79144	5.626595
H61	-1.7491	-2.70562	5.411886
H62	-0.22689	-3.53728	4.97726
H63	-0.54524	-3.05372	6.676229
H64	0.954473	-1.56701	5.682003

Table S141. [$Rh^{III}(ONN^{NMe_2})(TFA)_2(CH_3^{ax})]^-$

Atom	x	y	z
Rh1	0.476697	-0.00051	-0.0623
N2	0.135457	-0.37214	1.817727
C3	1.101549	-0.02529	2.688097
C4	0.941193	-0.21944	4.089184
C5	-0.34223	-0.73523	4.518413
C6	-1.29478	-1.07966	3.5669
C7	-1.03383	-0.89322	2.188291

C8	2.050158	0.080838	4.904425
H10	-2.26142	-1.45922	3.873462
C11	2.292325	0.511929	2.056023
C12	3.350533	0.821512	2.938956
C13	-1.9345	-1.13517	1.053151
O14	2.329182	0.653841	0.771472
N15	-1.45446	-0.8524	-0.12843
C16	0.701754	1.246194	-2.8666
O17	1.0521	0.320851	-2.05227
O18	-0.22003	2.05277	-2.84819
C19	1.66212	1.25941	-4.0949
F20	1.347575	2.22716	-4.97913
F21	2.948571	1.456179	-3.73041
F22	1.616557	0.081275	-4.77014
C23	3.210642	0.589164	4.309874
H24	4.268662	1.228638	2.528488
H25	4.059379	0.812633	4.954067
H26	2.021551	-0.1166	5.969003
C27	-3.59501	-1.19563	-3.73548
C28	-3.29474	-2.34603	-3.00501
C29	-2.60073	-2.24755	-1.79813
C30	-2.21101	-0.98825	-1.3265
C31	-2.49205	0.170192	-2.06137
C32	-3.19007	0.054786	-3.26103
H33	-4.12698	-1.2746	-4.68025
H34	-3.58849	-3.32414	-3.37754
H35	-2.3363	-3.13751	-1.23378
H36	-2.12959	1.128101	-1.70218
H37	-3.3959	0.952974	-3.83595
C38	-3.33801	-1.61289	1.316396
H39	-3.93742	-1.61472	0.407079
H40	-3.33178	-2.62694	1.733573
H41	-3.8148	-0.95749	2.053493
O42	-0.73982	1.856621	0.222517
C43	-0.32468	3.064248	0.152469
O44	0.801124	3.543298	0.16898
C45	-1.53298	4.050588	0.090629
F46	-1.16161	5.32272	-0.15312
F47	-2.43672	3.713367	-0.86102
F48	-2.20803	4.062744	1.276234

C49	1.361738	-1.84124	-0.34579
H50	1.142685	-2.14826	-1.37123
H51	2.438102	-1.70723	-0.21384
H52	0.982129	-2.58462	0.366248
N53	-0.57662	-0.90405	5.903862
C54	-1.63694	-1.81695	6.291834
H55	-1.5363	-2.76055	5.74887
H56	-1.54723	-2.02458	7.36383
H57	-2.65408	-1.41948	6.116829
C57	-0.6083	0.328059	6.697765
H58	-1.58053	0.84383	6.613204
H59	-0.43746	0.089792	7.754143
H60	0.169591	1.013562	6.364185

Table S142. $Rh^{III}(ONN^{NMe2})(TFA)(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.526644	-0.11452	-0.16945
N2	0.176265	-0.25703	1.736469
C3	1.177257	0.12274	2.557613
C4	1.034686	0.061353	3.970869
C5	-0.2674	-0.34485	4.468713
C6	-1.24957	-0.7461	3.556659
C7	-1.00251	-0.69857	2.1688
C8	2.187662	0.354101	4.731004
H10	-2.22529	-1.05352	3.90826
C11	2.374022	0.535988	1.863011
C12	3.468716	0.85115	2.679707
C13	-1.9275	-1.03046	1.065103
O14	2.376942	0.584116	0.550749
N15	-1.45098	-0.86918	-0.14149
C16	1.615926	0.793079	-2.83454
O17	0.898717	-0.06432	-2.24381
O18	2.039958	1.897917	-2.44733
C19	2.008815	0.36165	-4.27159
F20	2.713866	1.304766	-4.90901
F21	2.752913	-0.76168	-4.23253
F22	0.905105	0.101488	-5.00272
C23	3.356964	0.735425	4.074389
H24	4.400416	1.159843	2.21752
H25	4.2378	0.947607	4.675469

H26	2.184702	0.244046	5.807602
C27	-3.47341	-1.7054	-3.7396
C28	-3.24593	-2.73292	-2.82416
C29	-2.60127	-2.46876	-1.61533
C30	-2.18146	-1.16494	-1.32677
C31	-2.38831	-0.13476	-2.25255
C32	-3.04477	-0.40781	-3.44889
H33	-3.97015	-1.91596	-4.68212
H34	-3.56088	-3.74702	-3.05242
H35	-2.39604	-3.26941	-0.91101
H36	-2.02684	0.861844	-2.02233
H37	-3.20851	0.393323	-4.16361
C38	-3.33018	-1.469	1.380464
H39	-3.94983	-1.50721	0.485496
H40	-3.33019	-2.46128	1.84632
H41	-3.78033	-0.77246	2.095534
O42	-0.38686	2.073754	-0.01194
C43	0.232206	3.137909	-0.03137
O44	1.31644	3.428027	-0.65837
C45	-0.30374	4.339237	0.783132
F46	-0.5668	5.37866	-0.02753
F47	-1.43054	4.016761	1.432891
F48	0.608749	4.730023	1.690187
C49	1.269422	-2.01423	-0.21054
H50	1.114787	-2.37787	-1.22823
H51	2.334066	-1.94533	0.021665
H52	0.757415	-2.65315	0.515197
H53	1.634288	2.665033	-1.32435
N54	-0.50183	-0.37714	5.843809
C55	-0.29971	0.850896	6.621594
H56	0.454774	1.482778	6.158284
H57	-1.23495	1.428957	6.688445
H58	0.023051	0.602019	7.638284
C58	-1.62554	-1.15832	6.335926
H59	-1.50812	-1.2937	7.415207
H60	-2.60256	-0.67441	6.164561
H61	-1.63388	-2.14563	5.867422

Table S143. $Rh^{III}(ONN^{NMe2})(TFA)(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z

Rh1	0.452822	0.054869	-0.06522
N2	0.160834	-0.31349	1.819854
C3	1.164503	0.026035	2.655144
C4	1.054935	-0.1742	4.058148
C5	-0.21975	-0.67637	4.538254
C6	-1.2064	-1.02684	3.610384
C7	-0.99255	-0.8362	2.229144
C8	2.210572	0.095983	4.822512
H9	-2.16286	-1.40195	3.949065
C10	2.325859	0.560621	1.983539
C11	3.423971	0.844261	2.807002
C12	-1.93404	-1.08217	1.116629
O13	2.294904	0.742464	0.68334
N14	-1.49502	-0.77408	-0.07562
C15	1.416768	1.343022	-2.61487
O16	0.769638	0.374015	-2.12393
O17	1.789038	2.412867	-2.09785
C18	1.786053	1.125389	-4.10543
F19	2.424634	2.179631	-4.62853
F20	2.584088	0.04688	-4.23466
F21	0.673782	0.90723	-4.8375
C22	3.348125	0.58994	4.185701
H23	4.330094	1.240247	2.360787
H24	4.231466	0.78387	4.789307
H25	2.234604	-0.11429	5.883603
C26	-3.57405	-1.28295	-3.7025
C27	-3.29629	-2.39524	-2.90789
C28	-2.63311	-2.24222	-1.68989
C29	-2.24517	-0.96428	-1.2702
C30	-2.50337	0.152446	-2.07501
C31	-3.17782	-0.01113	-3.28118
H32	-4.08469	-1.4067	-4.65297
H33	-3.58598	-3.38842	-3.23865
H34	-2.38844	-3.10707	-1.08043
H35	-2.16653	1.129532	-1.74549
H36	-3.38068	0.856613	-3.90192
C37	-3.31309	-1.60089	1.413953
H38	-3.95417	-1.56422	0.534093
H39	-3.26923	-2.63678	1.76986
H40	-3.76688	-1.00101	2.209808

O41	-0.55589	2.158522	0.38292
C42	0.039628	3.227058	0.526892
O43	1.089856	3.649264	-0.08232
C44	-0.51737	4.260034	1.535328
F45	-1.32309	3.664361	2.427883
F46	0.468246	4.875439	2.203784
F47	-1.23353	5.194003	0.879872
C48	1.267238	-1.79323	-0.34775
H49	1.090863	-2.04556	-1.39521
H50	2.33583	-1.70488	-0.14191
H51	0.806638	-2.53125	0.315661
H52	1.399874	3.005798	-0.86758
N53	-0.42252	-0.8436	5.909357
C54	-0.26302	0.322814	6.786542
H55	0.465721	1.018865	6.377021
H56	-1.21879	0.858122	6.902673
H57	0.073039	0.001506	7.778193
C58	-1.50811	-1.70829	6.344955
H59	-1.36757	-1.93437	7.406114
H60	-2.50509	-1.24865	6.230985
H61	-1.48798	-2.64946	5.789875

Table S144. $Rh^{II}(ONN^{NMe_2})(TFA)$

Atom	x	y	z
Rh1	0.473032	-0.19157	-0.18307
N2	-0.0695	-0.35399	1.69104
C3	0.796069	0.136747	2.606392
C4	0.504771	0.099619	3.997696
C5	-0.79636	-0.42416	4.369744
C6	-1.62731	-0.9473	3.372584
C7	-1.23998	-0.90274	2.017871
C8	1.531711	0.526936	4.86791
H10	-2.5983	-1.34913	3.629261
C11	2.026659	0.628365	2.031809
C12	2.98467	1.080137	2.950359
C13	-2.00549	-1.36094	0.840386
O14	2.189985	0.597072	0.730597
N15	-1.4311	-1.17019	-0.31859
C16	0.417724	1.218661	-2.37281
O17	1.045022	0.127392	-2.22309

O18	-0.2872	1.752094	-1.48619
C19	0.462006	1.89343	-3.75788
F20	-0.72579	1.700099	-4.38339
F21	0.652336	3.218273	-3.64437
F22	1.425862	1.394838	-4.54217
C23	2.726368	1.001286	4.328197
H24	3.93285	1.456273	2.580938
H25	3.50941	1.318624	5.012684
H26	1.417954	0.448262	5.941276
C27	-2.98327	-2.41281	-4.03505
C28	-2.63836	-3.36575	-3.07596
C29	-2.15105	-2.96719	-1.83131
C30	-2.00957	-1.60323	-1.54806
C31	-2.34107	-0.64329	-2.51212
C32	-2.83318	-1.05414	-3.74864
H33	-3.35368	-2.72737	-5.00631
H34	-2.73759	-4.42441	-3.29772
H35	-1.85358	-3.70446	-1.09119
H36	-2.19248	0.407777	-2.28941
H37	-3.08053	-0.30587	-4.49565
C38	-3.368	-1.96713	1.032467
H39	-3.8778	-2.11764	0.081802
H40	-3.29221	-2.93378	1.543848
H41	-3.97789	-1.31188	1.66345
N42	-1.17711	-0.44685	5.712233
C43	-2.26116	-1.33119	6.109874
H44	-2.11686	-2.32453	5.677749
H45	-2.24778	-1.42827	7.199613
H46	-3.25876	-0.9582	5.820359
C46	-1.18866	0.814206	6.462514
H47	-0.95767	0.625722	7.516552
H48	-0.4549	1.50971	6.061011
H49	-2.17946	1.292575	6.407145

Table S145. $[Rh^{III}(ONN^{NMe_2})(TFA^{ax})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	0.373063	-0.10101	-0.17951
N2	0.100066	-0.36734	1.729289
C3	1.1187	0.011143	2.525676
C4	1.021866	-0.10039	3.939273

C5	-0.25626	-0.55194	4.462066
C6	-1.25674	-0.94943	3.564866
C7	-1.05771	-0.8396	2.176298
C8	2.195384	0.192335	4.668911
N9	-0.45535	-0.63091	5.837285
H10	-2.21906	-1.27761	3.933224
C11	2.278689	0.474876	1.807016
C12	3.39386	0.785831	2.593234
C13	-2.02599	-1.10782	1.091627
O14	2.237126	0.560604	0.493595
N15	-1.59625	-0.89393	-0.12275
C16	1.631578	-0.18992	-2.76419
O17	0.625339	0.347884	-2.24089
O18	2.35298	-1.08031	-2.24195
C19	2.041363	0.277806	-4.17647
F20	3.228016	0.905309	-4.11696
F21	2.16459	-0.78289	-4.99457
F22	1.143305	1.115365	-4.70586
C23	3.332258	0.620466	3.986852
H24	4.301841	1.131698	2.11141
H25	4.228242	0.832471	4.564626
H26	2.231958	0.048884	5.740932
C27	-3.73162	-1.56444	-3.68892
C28	-3.49753	-2.62711	-2.81622
C29	-2.81351	-2.41451	-1.6195
C30	-2.36331	-1.12737	-1.29825
C31	-2.57589	-0.06044	-2.18178
C32	-3.2709	-0.28531	-3.36718
H33	-4.25984	-1.73366	-4.62256
H34	-3.83785	-3.62723	-3.06832
H35	-2.60575	-3.24162	-0.94688
H36	-2.19073	0.924063	-1.93894
H37	-3.44094	0.543129	-4.04827
C38	-3.42513	-1.51721	1.446994
H39	-4.05888	-1.6077	0.566654
H40	-3.42821	-2.47108	1.986158
H41	-3.84697	-0.75489	2.111361
O53	-0.31624	1.837737	-0.16534
C54	-1.27197	2.326846	0.54709
O55	-1.93526	1.83295	1.450001

C56	-1.60875	3.765049	0.059492
F57	-0.51103	4.519385	-0.1144
F58	-2.25492	3.690501	-1.13075
F59	-2.41637	4.400241	0.921842
C60	1.122777	-2.30204	-0.28453
H61	0.42138	-2.87044	-0.89817
H62	2.118447	-2.7604	-0.37013
H63	0.873512	-2.40879	0.769056
H64	1.721489	-1.43217	-1.13185
C55	-1.55768	-1.43888	6.33636
H56	-1.40578	-1.6089	7.406289
H57	-2.54202	-0.9573	6.210091
H58	-1.57236	-2.41053	5.836227
C58	-0.22346	0.560025	6.663825
H59	0.165853	0.267827	7.645133
H60	0.487445	1.23088	6.187214
H65	-1.16317	1.112982	6.815065

Table S146. [$Rh^{III}(ONN^{NMe2})(TFA^{ax})(CH_3^{eq}$-H-$TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	0.20907	0.175372	-0.31591
N2	0.017398	-0.34305	1.584737
C3	1.028043	0.039605	2.384727
C4	1.040716	-0.30909	3.762401
C5	-0.12969	-1.01377	4.254175
C6	-1.12787	-1.39838	3.347624
C7	-1.02583	-1.05013	1.988075
C8	2.214139	0.016488	4.480061
N9	-0.22187	-1.34557	5.603834
H10	-1.99817	-1.93872	3.693871
C11	2.075919	0.75923	1.702209
C12	3.192669	1.08266	2.478489
C13	-1.95801	-1.36998	0.881439
O14	1.940896	1.060853	0.423878
N15	-1.64727	-0.89957	-0.29272
C23	3.243081	0.690906	3.828654
H24	4.02363	1.606928	2.018671
H25	4.145986	0.917768	4.390159
H26	2.340654	-0.29662	5.508319
C27	-3.71408	-1.81803	-3.84544

C28	-2.9547	-2.79862	-3.20521
C29	-2.28688	-2.51088	-2.01506
C30	-2.38596	-1.22625	-1.46688
C31	-3.13335	-0.23351	-2.10988
C32	-3.80254	-0.53766	-3.29444
H33	-4.22815	-2.04732	-4.77439
H34	-2.87359	-3.79283	-3.63541
H35	-1.66909	-3.25165	-1.517
H36	-3.18195	0.761431	-1.67797
H37	-4.38798	0.230547	-3.79144
C38	-3.15987	-2.22311	1.157049
H39	-3.86143	-2.214	0.323885
H40	-2.83265	-3.25558	1.326253
H41	-3.67045	-1.88001	2.061818
O53	-0.8486	1.938017	0.187188
C54	-0.50068	2.95049	-0.46608
O55	0.255588	2.963228	-1.47703
C56	-1.06411	4.319688	-0.03759
F57	-0.0654	5.196836	0.132369
F58	-1.88315	4.784113	-0.99877
F59	-1.75703	4.232498	1.103063
O60	1.387795	-1.44946	-0.71981
C61	1.15009	-2.67605	-0.40329
O62	0.188966	-3.19053	0.157247
C63	2.310668	-3.58954	-0.89399
F64	2.232559	-4.80998	-0.34146
F65	2.237214	-3.73883	-2.23578
F66	3.51819	-3.0773	-0.59967
H67	0.450759	1.800983	-1.76555
C50	0.472691	0.586547	-2.54409
H51	1.237139	1.192892	-3.0516
H52	0.851471	-0.43131	-2.62209
H53	-0.47103	0.669282	-3.09073
C55	-1.15991	-2.38311	6.004226
H56	-0.91069	-2.70211	7.020588
H57	-2.20976	-2.0433	6.008418
H58	-1.07086	-3.24922	5.344089
C58	-0.10443	-0.28323	6.60828
H59	-1.09841	0.10463	6.881717
H60	0.37251	-0.67212	7.514481

H61	0.487832	0.545887	6.227544

Table S147. [$Rh^{III\text{-}I}(ONN^{NMe2})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Atom	x	y	z
Rh1	0.91724	0.022034	-0.07054
N2	0.339166	0.017514	1.774352
C3	1.172781	0.582444	2.681335
C4	0.766166	0.806314	4.022395
C5	-0.61028	0.49758	4.338732
C6	-1.41382	-0.10155	3.377225
C7	-0.91687	-0.34158	2.075871
C8	1.735632	1.322513	4.910183
N9	-1.10119	0.842031	5.622512
H10	-2.45236	-0.32269	3.589646
C11	2.462499	0.954486	2.138063
C12	3.37604	1.476691	3.074132
C13	-1.65506	-0.83466	0.906446
O14	2.696967	0.797568	0.866948
N15	-0.99741	-0.78276	-0.22425
C16	0.885075	1.229719	-2.75584
O17	1.407769	0.274261	-2.12375
O18	0.139173	2.15486	-2.36465
C19	1.216516	1.281096	-4.2695
F20	1.892914	2.415089	-4.56307
F21	1.964288	0.245703	-4.68351
F22	0.083263	1.285826	-5.00456
C23	3.003429	1.629933	4.417651
H24	4.367204	1.760312	2.734254
H25	3.746202	2.017889	5.112627
H26	1.501208	1.448464	5.960508
C27	-2.58698	-1.9653	-3.94518
C28	-1.82278	-2.85999	-3.19375
C29	-1.30839	-2.48818	-1.95068
C30	-1.58049	-1.20496	-1.46019
C31	-2.34145	-0.29698	-2.206
C32	-2.84143	-0.68568	-3.44845
H33	-2.97189	-2.25932	-4.91842
H34	-1.60973	-3.85483	-3.5757
H35	-0.69059	-3.18015	-1.3822
H36	-2.50962	0.700003	-1.81173

H37	-3.42345	0.021926	-4.03319
C38	-3.07966	-1.29137	1.038322
H39	-3.39281	-1.8613	0.163416
H40	-3.20863	-1.90874	1.932745
H41	-3.73377	-0.41552	1.130805
O42	-2.50404	2.220238	0.050393
C43	-1.57939	2.90167	0.450979
O44	-0.42944	3.155085	-0.10848
C45	-1.69231	3.639084	1.811145
F46	-1.83467	4.968325	1.618624
F47	-2.76305	3.209508	2.503333
F48	-0.60445	3.448326	2.579875
C49	1.959147	-2.16719	-0.16259
H50	1.802789	-2.06557	-1.22526
H51	2.848544	-1.75529	0.289394
H52	1.194659	-2.61765	0.447116
H53	-0.25382	2.649006	-0.99789
O54	2.856782	-3.87649	-0.42945
C55	2.031338	-4.82233	-0.66772
O56	0.800744	-4.82285	-0.71018
C57	2.774999	-6.16591	-0.93488
F58	3.620121	-6.06085	-1.98549
F59	3.512055	-6.54086	0.136914
F60	1.924382	-7.17426	-1.20613
C62	-2.2953	0.146438	6.073543
H63	-2.43212	0.339276	7.143198
H64	-3.21961	0.468133	5.559118
H65	-2.1765	-0.93094	5.930235
C65	-1.20487	2.289383	5.854277
H66	-2.0533	2.72956	5.303599
H67	-1.34534	2.477238	6.924697
H68	-0.2949	2.790393	5.525439

Table S148. [$Rh^{III-II}(ONN^{NMe2})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Atom	x	y	z
Rh1	0.887134	0.707622	0.871809
N2	-0.00319	0.572341	2.596268
C3	0.42526	1.412096	3.561517
C4	-0.17352	1.446403	4.845791
C5	-1.32284	0.575772	5.043483

C6	-1.66722	-0.32535	4.009113
C7	-0.99598	-0.30201	2.783404
C8	0.473483	2.268056	5.803772
H10	-2.49621	-1.00624	4.136693
C11	1.572524	2.185543	3.168959
C12	2.13587	3.011126	4.145433
C13	-1.2513	-1.13495	1.583872
O14	2.046549	2.038484	1.942649
N15	-0.48886	-0.87826	0.55328
C16	2.403186	1.756268	-1.49607
O17	1.976246	0.711372	-0.92619
O18	2.10869	2.95189	-1.29979
C19	3.411995	1.48542	-2.6419
F20	4.255902	2.513411	-2.80095
F21	4.134776	0.378487	-2.41498
F22	2.734296	1.313976	-3.79759
C23	1.587284	3.019063	5.439732
H24	3.008939	3.606596	3.900657
H25	2.066992	3.630784	6.198441
H26	0.142608	2.289521	6.832985
C27	-0.48896	-2.97646	-3.09367
C28	-0.19923	-3.65658	-1.91073
C29	-0.22665	-2.98704	-0.68702
C30	-0.53776	-1.62211	-0.66307
C31	-0.80428	-0.92595	-1.84953
C32	-0.79442	-1.61288	-3.05946
H33	-0.4619	-3.50254	-4.04341
H34	0.068065	-4.70831	-1.93123
H35	0.033952	-3.50701	0.229632
H36	-1.01673	0.137006	-1.80489
H37	-1.0101	-1.07829	-3.97989
C38	-2.32459	-2.18154	1.616118
H39	-2.56978	-2.52801	0.612678
H40	-1.98707	-3.04233	2.205229
H41	-3.22712	-1.78061	2.087476
O42	-0.90795	2.047812	0.055746
C43	-0.83546	3.280926	0.048927
O44	0.174514	4.021979	-0.22943
C45	-2.09029	4.07242	0.487305
F46	-3.2	3.498201	0.000664

F47	-2.16255	4.045328	1.836992
F48	-2.05985	5.348103	0.093879
C49	2.485365	-1.10217	1.355404
H50	2.419127	-1.45766	0.337607
H51	3.231773	-0.36034	1.601911
H52	1.78441	-1.43827	2.101872
H53	1.01797	3.474297	-0.60045
O54	3.651731	-2.56894	1.936514
Cl55	4.371567	-5.33827	3.580279
Cl56	1.078401	-3.83686	3.084385
Cl57	2.737146	-5.12024	0.303363
V59	3.157038	-4.10184	2.235182
N59	-2.04683	0.582757	6.20957
C60	-2.3495	1.812796	6.945217
H61	-1.95365	2.683046	6.425777
H62	-3.43799	1.929457	7.014406
H63	-1.94407	1.784591	7.963681
C63	-2.94695	-0.52232	6.518513
H64	-3.90498	-0.45131	5.980981
H65	-2.47466	-1.47868	6.283764
H66	-3.15794	-0.50674	7.59053

Rh(DPMS) complexes in TFAH

Table S149. [Rh^{I}(DPMS)(TFA)(TFAH)]$^{-}$

Atom	x	y	z
Rh1	0.026775	-0.0375	0.011498
N2	0.004338	-0.02197	2.045518
C3	1.193979	-0.0561	2.698351
C4	1.302754	0.028178	4.075479
C5	0.138578	0.169132	4.833359
C6	-1.07769	0.196999	4.171186
C7	-1.13512	0.081185	2.772071
C8	-2.48653	0.1076	2.130423
C9	-2.7383	-0.75434	0.934872
C10	-4.00955	-1.3387	0.806151
C11	-4.30639	-2.15325	-0.27417
C12	-3.31246	-2.37599	-1.22943
C13	-2.08535	-1.75713	-1.06757

N14	-1.79381	-0.9492	-0.01671
H15	2.067073	-0.11532	2.063835
H16	2.285285	-0.00439	4.535242
H17	0.180439	0.258894	5.915317
H18	-2.00644	0.339778	4.710304
H19	-3.1961	-0.21163	2.895805
H20	-4.75616	-1.10706	1.556081
H21	-5.29028	-2.60328	-0.37283
H22	-3.48053	-3.00896	-2.09483
H23	-1.29827	-1.865	-1.80031
S24	-3.13407	1.896342	1.868093
O25	-4.52074	1.634508	1.486175
O26	-2.9634	2.456046	3.207275
O27	-2.29334	2.471508	0.829213
O28	1.964674	0.856143	0.101604
C29	2.371454	1.959765	-0.31738
O30	1.896458	2.730504	-1.19237
C31	3.697614	2.46869	0.301378
F32	4.683073	2.459032	-0.62549
F33	3.571947	3.731557	0.748421
F34	4.109121	1.708916	1.334106
O35	-0.02674	-0.06005	-2.14294
C36	-0.06423	0.846018	-2.98337
O37	0.335729	2.056993	-2.90542
C38	-0.63416	0.499497	-4.37743
F39	0.366015	0.437658	-5.28476
F40	-1.25807	-0.69018	-4.37615
F41	-1.50978	1.428515	-4.79374
H42	0.96191	2.31114	-2.01507

Table S150. $Rh^{I}(DPMS)(TFAH)_2$

Atom	x	y	z
Rh1	0.086853	-0.25947	0.006983
N2	0.034926	-0.2185	2.029891
C3	1.129687	-0.50464	2.770415
C4	1.149661	-0.37246	4.151486
C5	-0.0003	0.076932	4.800584
C6	-1.1285	0.362431	4.039216
C7	-1.09422	0.199415	2.651394
C8	-2.32349	0.489975	1.825864

C9	-2.70356	-0.59185	0.844953
C10	-4.01925	-1.06136	0.795003
C11	-4.3631	-2.07173	-0.09657
C12	-3.37349	-2.59811	-0.92674
C13	-2.08695	-2.08549	-0.84188
N14	-1.75514	-1.09734	0.019813
H15	1.996914	-0.83647	2.212745
H16	2.052799	-0.61663	4.700099
H17	-0.01862	0.202325	5.878722
H18	-2.03646	0.728342	4.505512
H19	-3.15765	0.58887	2.525552
H20	-4.76372	-0.6164	1.445767
H21	-5.38292	-2.44081	-0.14221
H22	-3.58821	-3.39238	-1.63329
H23	-1.28206	-2.44638	-1.4705
S24	-2.36996	2.222481	1.10971
O25	-3.66633	2.28227	0.476688
O26	-2.08796	3.058193	2.252752
O27	-1.25919	2.334899	0.073278
O28	1.972963	0.768269	0.041643
C29	2.102916	1.970483	0.28591
O30	1.198437	2.873315	0.477518
C31	3.526303	2.559365	0.399734
F32	3.709279	3.506994	-0.5326
F33	3.69331	3.113943	1.61216
F34	4.450518	1.60954	0.234396
O35	0.029848	-0.18631	-2.13878
C36	-0.63236	0.628224	-2.78682
O37	-1.33741	1.629397	-2.37415
C38	-0.68187	0.494952	-4.32479
F39	-0.20083	1.607312	-4.90073
F40	0.040674	-0.54988	-4.73706
F41	-1.95337	0.321588	-4.72412
H42	-1.33658	1.812728	-1.35787
H43	0.214418	2.573888	0.386194

Table S151. [Rh^{III}(DPMS)$(TFA)_3$($TFAH^{eq}$)]$^-$

Atom	x	y	z
Rh1	0.140657	0.075537	-0.09077
N2	0.08861	0.234524	1.952033

C3	1.279915	0.487415	2.542166
C4	1.409742	0.641695	3.908745
C5	0.267577	0.533264	4.70306
C6	-0.94231	0.247669	4.098089
C7	-1.02375	0.08571	2.702212
C8	-2.36447	-0.26001	2.142073
C9	-2.48144	-1.02227	0.860468
C10	-3.68258	-1.72626	0.657198
C11	-3.83212	-2.57128	-0.4272
C12	-2.75922	-2.74105	-1.30263
C13	-1.60531	-2.01086	-1.08719
N14	-1.48607	-1.14967	-0.04681
H15	2.126491	0.568188	1.878888
H16	2.387954	0.84757	4.328836
H17	0.322496	0.661847	5.780239
H18	-1.86295	0.180015	4.664584
H19	-2.83384	-0.90798	2.884439
H20	-4.48808	-1.56005	1.360671
H21	-4.76674	-3.10387	-0.57903
H22	-2.80509	-3.41667	-2.14946
H23	-0.73863	-2.10312	-1.72534
S24	-3.61119	1.233943	2.382085
O25	-4.74999	0.831308	1.569021
O26	-3.82409	1.134521	3.825288
O27	-2.89035	2.419655	1.953382
O28	1.908717	1.306539	-0.11909
C29	2.223745	2.418574	-0.56435
O30	1.810582	3.033378	-1.59968
C31	3.373043	3.157019	0.161391
F32	4.530892	2.92404	-0.49528
F33	3.169761	4.477058	0.194005
F34	3.518632	2.715598	1.420086
O35	0.163249	-0.1672	-2.18698
C36	0.039656	0.682038	-3.10777
O37	0.317039	1.898695	-3.14029
C38	-0.48188	0.090565	-4.44503
F39	0.563466	-0.25937	-5.22558
F40	-1.23497	-1.00645	-4.25089
F41	-1.21981	0.984151	-5.11998
H42	1.081667	2.489991	-2.20112

O43	-1.23336	1.537993	-0.42758
C44	-1.05992	2.754782	-0.00547
O45	-0.14175	3.221494	0.64945
C46	-2.13431	3.711848	-0.58718
F47	-1.64301	4.214899	-1.75583
F48	-3.30102	3.121908	-0.87038
F49	-2.36276	4.74996	0.225526
O50	1.560615	-1.39786	0.280902
C51	1.871919	-2.39627	-0.47185
O52	1.320669	-2.86657	-1.45572
C53	3.185007	-3.05646	0.042231
F54	3.538087	-4.11421	-0.70621
F55	4.213118	-2.1792	0.018121
F56	3.051581	-3.48778	1.31732

Table S152. [Rh^{III}(DPMS)(TFA)$_3$]$^-$

Atom	x	y	z
Rh1	0.017853	-0.02336	0.031749
N2	-0.03164	0.011179	2.118237
C3	1.097621	0.168771	2.832518
C4	1.062755	0.328863	4.214116
C5	-0.16829	0.342742	4.863243
C6	-1.33008	0.198244	4.110259
C7	-1.23667	0.035454	2.727759
C8	-2.46893	-0.06317	1.866165
C9	-2.50366	-1.28637	0.988567
C10	-3.51312	-2.24184	1.106491
C11	-3.49523	-3.36011	0.277017
C12	-2.46955	-3.49351	-0.65459
C13	-1.48996	-2.50782	-0.73192
N14	-1.52097	-1.43342	0.07785
H15	2.019026	0.14662	2.262477
H16	1.994337	0.446541	4.756513
H17	-0.22726	0.471729	5.940425
H18	-2.309	0.226919	4.576235
H19	-3.35145	-0.06378	2.50851
H20	-4.29801	-2.09973	1.841747
H21	-4.27312	-4.11435	0.359553
H22	-2.41573	-4.34602	-1.32275
H23	-0.67214	-2.53465	-1.44951

S24	-2.66919	1.491193	0.853553
O25	-3.7917	1.208482	-0.01604
O26	-2.83545	2.540398	1.83798
O27	-1.35304	1.596149	0.132413
O28	1.473963	1.390124	0.189405
C29	2.525927	1.43422	-0.56439
O30	2.887652	0.729047	-1.48687
C31	3.420342	2.624198	-0.10952
F32	4.558498	2.692468	-0.82036
F33	2.785204	3.80855	-0.24627
F34	3.766796	2.503635	1.195618
O35	-0.02907	0.28236	-1.98902
C36	0.25292	-0.51961	-2.95024
O37	0.348778	-1.74145	-2.99062
C38	0.388818	0.250104	-4.29612
F39	1.235796	-0.37921	-5.13238
F40	-0.82172	0.294032	-4.91307
F41	0.814053	1.514475	-4.15678
O42	1.218811	-1.66467	-0.11861
C43	2.402034	-1.8544	0.351625
O44	3.111095	-1.16501	1.070481
C45	2.910927	-3.26113	-0.07992
F46	2.885388	-3.4285	-1.41046
F47	4.168572	-3.48043	0.341441
F48	2.130463	-4.22861	0.469761

Table S153. $Rh^{III}(DPMS)(TFA)_2(TFAH^{ax})$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.100839
C3	1.138541	0	2.814477
C4	1.140101	0.09824	4.199754
C5	-0.07965	0.216644	4.862848
C6	-1.25446	0.228864	4.117116
C7	-1.1906	0.116722	2.727495
C8	-2.42922	0.172683	1.873894
C9	-2.60924	-1.00622	0.955234
C10	-3.7268	-1.83667	1.019959
C11	-3.86236	-2.87441	0.101755
C12	-2.88462	-3.0484	-0.87598

C13	-1.79471	-2.18826	-0.89501
N14	-1.66447	-1.20774	0.014996
H15	2.060311	-0.05419	2.250071
H16	2.082433	0.094991	4.73617
H17	-0.11624	0.305559	5.944168
H18	-2.22066	0.337566	4.59718
H19	-3.30585	0.262182	2.517559
H20	-4.48193	-1.65711	1.777143
H21	-4.72653	-3.53068	0.140526
H22	-2.95926	-3.83018	-1.62341
H23	-1.02138	-2.24675	-1.64826
S24	-2.45537	1.749749	0.875854
O25	-3.57735	1.59346	-0.01388
O26	-2.47093	2.812127	1.850705
O27	-1.10592	1.709278	0.156884
O28	1.76582	1.104218	0.109376
C29	1.952357	2.262698	-0.52079
O30	1.23782	2.802525	-1.32083
C31	3.276513	2.909238	-0.03881
F32	3.586453	3.986422	-0.75793
F33	3.169052	3.274503	1.257098
F34	4.299374	2.025745	-0.12806
O35	-0.23458	0.00242	-2.01802
C36	0.762519	-0.13667	-2.82721
O37	1.957444	-0.24432	-2.58577
C38	0.245497	-0.26885	-4.28474
F39	1.248166	-0.22247	-5.16792
F40	-0.36975	-1.47686	-4.41262
F41	-0.64552	0.679835	-4.60164
H42	2.741815	0.031516	-0.0401
O50	1.133662	-1.77156	-0.15209
C51	2.37613	-1.84149	-0.1998
O52	3.227767	-0.8985	-0.05812
C53	2.985469	-3.25267	-0.35495
F54	4.215619	-3.20085	-0.8604
F55	3.038957	-3.82515	0.864459
F56	2.212845	-4.00598	-1.14356

Table S154. $Rh^{III}(DPMS)(TFA)_2(TFAH^{eq})$

Atom	x	y	z

Rh1	0	0	0
N2	0	0	2.056618
C3	1.150721	0	2.75611
C4	1.148584	0.103154	4.141982
C5	-0.06829	0.220539	4.809301
C6	-1.24928	0.220224	4.071656
C7	-1.19244	0.103673	2.683779
C8	-2.43562	0.1145	1.833303
C9	-2.55325	-1.0836	0.929465
C10	-3.65356	-1.93839	0.971739
C11	-3.71047	-3.02809	0.106974
C12	-2.66396	-3.24181	-0.78731
C13	-1.59431	-2.35639	-0.79436
N14	-1.55504	-1.30944	0.048831
H15	2.062491	-0.08391	2.175649
H16	2.092225	0.097578	4.675657
H17	-0.10003	0.312647	5.890643
H18	-2.21359	0.319835	4.557098
H19	-3.31265	0.160252	2.480755
H20	-4.4539	-1.73857	1.675207
H21	-4.56217	-3.70087	0.131868
H22	-2.66623	-4.07691	-1.47838
H23	-0.7567	-2.46209	-1.4679
S24	-2.54338	1.691739	0.844579
O25	-3.72006	1.529336	0.026379
O26	-2.51583	2.747365	1.826885
O27	-1.25743	1.650407	0.032894
O28	1.500836	1.474874	0.222642
C29	2.567477	1.829874	-0.29985
O30	3.081122	1.49382	-1.41538
C31	3.379695	2.870445	0.507211
F32	4.608467	3.035123	0.016802
F33	2.739389	4.049236	0.479162
F34	3.475357	2.469297	1.786045
O35	-0.23916	-0.08547	-2.06194
C36	0.657768	-0.26804	-2.93904
O37	1.878742	-0.04292	-2.89895
C38	0.094658	-0.91688	-4.23032
F39	0.994984	-0.94301	-5.21358
F40	-0.2593	-2.19642	-3.94822

F41	-0.9981	-0.27262	-4.66205
H42	2.507031	0.797255	-1.98111
O50	1.149933	-1.67861	-0.20972
C51	2.423418	-1.76156	0.013654
O52	3.179997	-0.94949	0.523366
C53	2.955469	-3.14663	-0.44857
F54	4.286778	-3.20834	-0.36597
F55	2.437996	-4.12187	0.330212
F56	2.595038	-3.40104	-1.72092

Table S155. $[Rh^{III}(DPMS)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})]^{+}$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.046066
C3	1.145974	0	2.753186
C4	1.147788	0.130932	4.135179
C5	-0.06964	0.283287	4.796561
C6	-1.24861	0.286435	4.054763
C7	-1.19504	0.137325	2.6703
C8	-2.44287	0.138223	1.824263
C9	-2.57362	-1.07737	0.945288
C10	-3.66518	-1.93869	1.008137
C11	-3.73613	-3.01826	0.129399
C12	-2.71364	-3.21112	-0.7981
C13	-1.64818	-2.32059	-0.81769
N14	-1.59126	-1.28659	0.043363
H15	2.065454	-0.08244	2.190214
H16	2.090168	0.125602	4.671018
H17	-0.1021	0.401505	5.875027
H18	-2.21111	0.412307	4.537849
H19	-3.31833	0.216488	2.47113
H20	-4.45191	-1.75348	1.730848
H21	-4.5825	-3.69677	0.165942
H22	-2.73298	-4.03435	-1.50321
H23	-0.82836	-2.41358	-1.51732
S24	-2.53431	1.664023	0.767481
O25	-3.5489	1.389503	-0.21341
O26	-2.65392	2.779488	1.66139
O27	-1.11478	1.671969	0.132033
O28	1.729797	1.190077	0.045317

C29	1.812982	2.436389	-0.33145
O30	1.076185	3.040854	-1.0962
C31	3.009652	3.161464	0.332829
F32	3.187773	4.373871	-0.16723
F33	2.783103	3.250219	1.655706
F34	4.127702	2.430426	0.144683
O35	-0.17339	-0.0481	-2.10004
C36	-0.60477	0.829444	-2.87954
O37	-0.55813	2.095858	-2.75999
C38	-1.24531	0.316184	-4.19308
F39	-1.94659	1.265515	-4.79673
F40	-0.26403	-0.10558	-5.00314
F41	-2.04766	-0.72056	-3.90826
H42	0.004733	2.440323	-1.9622
O50	1.229106	-1.71472	-0.18694
C51	2.45592	-1.7673	-0.37711
O52	3.295285	-0.79067	-0.36727
C53	3.068994	-3.16677	-0.62789
F54	4.350526	-3.08067	-0.95798
F55	2.938351	-3.88584	0.494522
F56	2.385721	-3.75998	-1.61253
H57	2.832	0.098094	-0.20302

Table S156. [Rh^{III}(DPMS)(TFA^{ax})($TFAH^{eq}$)$_2$]$^+$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.014658
C3	1.161523	0	2.694515
C4	1.178342	0.049958	4.081072
C5	-0.03456	0.107035	4.76641
C6	-1.22675	0.100732	4.045535
C7	-1.19003	0.040237	2.654359
C8	-2.43919	0.023771	1.811003
C9	-2.51331	-1.18009	0.907132
C10	-3.59981	-2.05211	0.917209
C11	-3.59477	-3.16751	0.082741
C12	-2.49251	-3.39928	-0.73815
C13	-1.43993	-2.49386	-0.72009
N14	-1.47058	-1.40689	0.074505
H15	2.066225	-0.04282	2.103551

H16	2.128065	0.046177	4.603623
H17	-0.05313	0.153389	5.850662
H18	-2.18511	0.146839	4.550308
H19	-3.31367	0.040131	2.463494
H20	-4.43733	-1.8494	1.575067
H21	-4.43685	-3.85218	0.082146
H22	-2.43785	-4.26586	-1.38714
H23	-0.5535	-2.63199	-1.32365
S24	-2.58841	1.600638	0.841473
O25	-3.84358	1.513598	0.144201
O26	-2.3567	2.652914	1.79234
O27	-1.421	1.457339	-0.15409
O28	1.369917	1.614755	0.127943
C29	2.152143	2.12042	-0.69515
O30	2.722314	1.551258	-1.6899
C31	2.465717	3.631202	-0.55835
F32	1.703416	4.28879	-1.44905
F33	2.175772	4.058204	0.667917
F34	3.750611	3.869522	-0.82258
O35	-0.16778	-0.11298	-2.15813
C36	-0.40716	0.765776	-2.97944
O37	-0.21321	2.035743	-2.75926
C38	-0.95159	0.348987	-4.37126
F39	-1.18092	1.458456	-5.10297
F40	-0.05661	-0.41223	-4.99265
F41	-2.09042	-0.32091	-4.21947
H42	2.624027	0.504863	-1.68496
H43	-0.48443	2.578641	-3.52315
O50	1.351824	-1.55283	0.034902
C51	2.249445	-1.73118	-0.86199
O52	2.711644	-0.92756	-1.68046
C53	2.729062	-3.20485	-0.92474
F54	3.795886	-3.34095	-1.703
F55	3.008029	-3.67098	0.29812
F56	1.716308	-3.94109	-1.44203

Table S157. $Rh^{III}(DPMS)(TFA^{eq})_2(TFAH^{ax})_2$

Atom	x	y	z
Rh1	0.005558	0.17477	0.014761
N2	0.044531	0.278907	2.082448

C3	1.244338	0.584359	2.633412
C4	1.462529	0.548371	3.996935
C5	0.40679	0.18056	4.833164
C6	-0.8162	-0.13063	4.266407
C7	-0.99015	-0.08025	2.872521
C8	-2.3497	-0.32337	2.334682
C9	-2.5455	-1.03771	1.03901
C10	-3.77996	-1.68695	0.85645
C11	-4.01807	-2.45313	-0.27008
C12	-3.00683	-2.58235	-1.22488
C13	-1.82539	-1.89527	-1.02654
N14	-1.60202	-1.13189	0.070177
H15	2.024158	0.877154	1.947626
H16	2.441446	0.805199	4.385237
H17	0.537392	0.141192	5.910005
H18	-1.67242	-0.38171	4.879412
H19	-2.89217	-0.91004	3.0755
H20	-4.54258	-1.54987	1.613088
H21	-4.97564	-2.94644	-0.40397
H22	-3.13305	-3.18004	-2.12039
H23	-1.04144	-1.90598	-1.76915
S24	-3.35447	1.349254	2.572193
O25	-4.53989	1.113248	1.769449
O26	-3.52486	1.319421	4.014226
O27	-2.44322	2.393611	2.097598
O28	1.420663	1.705916	0.00617
C29	2.531029	1.668819	-0.68879
O30	2.974922	0.742893	-1.33594
C31	3.333952	2.983111	-0.51322
F32	3.886572	2.989514	0.721308
F33	4.309208	3.084666	-1.41423
F34	2.535607	4.061758	-0.61446
O35	0.180417	-0.11875	-2.063
C36	0.192367	0.872397	-2.93653
O37	0.101644	2.057481	-2.71948
C38	0.297679	0.321993	-4.38272
F39	1.284113	-0.59763	-4.47071
F40	-0.85847	-0.28522	-4.72168
F41	0.542882	1.293461	-5.25748
O43	-1.49732	1.513144	-0.34214

C44	-1.47647	2.748565	-0.17386
O45	-0.46455	3.478478	0.132178
C46	-2.73681	3.554385	-0.56081
F47	-2.52656	4.015213	-1.81302
F48	-3.82023	2.789055	-0.5671
F49	-2.90978	4.594395	0.249015
O50	1.434187	-1.32723	0.339041
C51	2.025509	-1.99812	-0.52539
O52	1.880372	-1.9615	-1.79686
C53	3.026252	-3.05604	-0.00642
F54	3.749817	-3.57145	-0.9972
F55	3.841724	-2.49882	0.89499
F56	2.332711	-4.04164	0.588404
H42	0.382294	2.934973	0.138713
H57	1.250084	-1.19202	-2.07035

Table S158. $Rh^{III}(DPMS)(TFA^{ax})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})$

Atom	x	y	z
Rh1	-0.20758	0.154335	-0.01283
N2	0.017999	0.18987	2.009909
C3	1.262505	0.488038	2.460043
C4	1.557008	0.578554	3.8047
C5	0.5346	0.347475	4.72785
C6	-0.7193	-0.00571	4.263537
C7	-0.97313	-0.10571	2.882467
C8	-2.33944	-0.53433	2.470395
C9	-2.53622	-1.29635	1.200722
C10	-3.65648	-2.14348	1.120891
C11	-3.83959	-2.96766	0.024569
C12	-2.88723	-2.96112	-0.99796
C13	-1.82266	-2.08844	-0.89497
N14	-1.66828	-1.26354	0.166442
H15	2.020776	0.642941	1.708156
H16	2.566374	0.826698	4.111783
H17	0.719535	0.426054	5.79456
H18	-1.54595	-0.18501	4.940149
H19	-2.69285	-1.20301	3.256607
H20	-4.3748	-2.11515	1.930722
H21	-4.7073	-3.61742	-0.03053
H22	-2.96992	-3.60541	-1.86565

H23	-1.07213	-2.0141	-1.66883
S24	-3.62819	0.896233	2.826794
O25	-4.81736	0.405648	2.155586
O26	-3.63803	0.854101	4.279752
O27	-3.01965	2.104174	2.267819
O28	1.387498	1.459729	-0.37603
C29	1.671946	2.608697	0.101675
O30	0.962638	3.400791	0.729602
C31	3.168165	2.962105	-0.1076
F32	3.535241	2.775837	-1.38398
F33	3.436828	4.220215	0.239447
F34	3.91341	2.138068	0.668636
O35	-0.53701	0.20118	-2.14693
C36	0.143907	0.701519	-3.05913
O37	1.412983	0.696606	-3.19247
C38	-0.6422	1.424798	-4.17773
F39	0.164314	1.910927	-5.12098
F40	-1.50633	0.566521	-4.73928
F41	-1.33225	2.435971	-3.62868
H42	1.881918	0.104008	-2.45809
O43	-1.84558	1.420106	-0.17225
C44	-2.20432	2.594032	0.043973
O45	-1.51404	3.597669	0.42906
C46	-3.62169	2.970641	-0.44636
F47	-3.47691	3.415087	-1.7198
F48	-4.42898	1.914477	-0.46233
F49	-4.1596	3.944591	0.278959
O50	1.19411	-1.32988	0.09346
C51	2.224732	-1.47353	-0.64933
O52	2.55629	-0.90429	-1.69433
C53	3.178534	-2.55939	-0.07908
F54	4.237592	-2.74413	-0.86756
F55	3.61141	-2.17854	1.138332
F56	2.530181	-3.72992	0.050544
H57	-0.52232	3.401945	0.625364

Table S159. $Rh^{III}(DPMS)(TFA^{ax})_2(TFAH^{eq})_2$

Atom	x	y	z
Rh1	0.105067	0.186337	0.160584
N2	0.003896	0.415178	2.174903

C3	1.164176	0.801781	2.758436
C4	1.254815	1.069761	4.108164
C5	0.102495	0.95303	4.889465
C6	-1.06859	0.534743	4.288943
C7	-1.111	0.239469	2.913488
C8	-2.39807	-0.26312	2.375719
C9	-2.4537	-1.0816	1.145798
C10	-3.52399	-1.9903	1.027432
C11	-3.71625	-2.71148	-0.13412
C12	-2.83715	-2.51384	-1.2023
C13	-1.80038	-1.61889	-1.04212
N14	-1.60195	-0.92878	0.108536
H15	2.022581	0.896525	2.110179
H16	2.207472	1.372301	4.527594
H17	0.123883	1.177925	5.951175
H18	-1.98825	0.443594	4.852975
H19	-2.86228	-0.83892	3.176093
H20	-4.21058	-2.07277	1.859983
H21	-4.54277	-3.41033	-0.21437
H22	-2.94739	-3.0386	-2.14421
H23	-1.10528	-1.42289	-1.84298
S24	-3.77416	1.13688	2.196654
O25	-4.97373	0.315982	2.2256
O26	-3.5246	1.95153	3.370639
O27	-3.46618	1.735904	0.901595
O28	2.002203	1.238787	0.009478
C29	2.188106	2.235833	-0.70858
O30	1.306264	2.910645	-1.35058
C31	3.650871	2.688758	-0.9125
F32	4.247711	1.807391	-1.73451
F33	3.723244	3.903654	-1.44861
F34	4.289231	2.681837	0.263099
O35	0.473696	0.07218	-2.00965
C36	1.430824	-0.51591	-2.53651
O37	2.190158	-1.41152	-2.01063
C38	1.814231	-0.10432	-3.97618
F39	0.713013	0.104	-4.70064
F40	2.510513	1.04487	-3.89776
F41	2.566646	-1.02897	-4.57052
H42	0.360314	2.553292	-1.1278

O43	-0.83942	1.92174	-0.39641
C44	-1.21713	2.893868	0.447432
O45	-0.81337	3.080349	1.567852
C46	-2.0655	3.95492	-0.29957
F47	-1.17351	4.764747	-0.9458
F48	-2.87812	3.44347	-1.22463
F49	-2.76357	4.702667	0.546719
O50	1.270517	-1.53553	0.33369
C51	1.087624	-2.51685	1.194527
O52	0.222349	-2.61877	2.032354
C53	2.20174	-3.58965	1.061771
F54	1.842295	-4.73198	1.644388
F55	2.473	-3.84059	-0.23974
F56	3.333419	-3.14641	1.640583
H57	1.918512	-1.59601	-1.03119

Table S160. [Rh^{III}(DPMS)(TFA^{ax})$_2$($TFAH^{eq}$)(CH_3^{ax})]$^-$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.037444
C3	1.21302	0	2.631797
C4	1.39367	-0.41063	3.940474
C5	0.282447	-0.87327	4.644177
C6	-0.9696	-0.79676	4.055048
C7	-1.115	-0.27796	2.756657
C8	-2.49887	0.062223	2.284574
C9	-2.78073	0.567851	0.902594
C10	-4.11854	0.822493	0.555226
C11	-4.42391	1.525486	-0.5995
C12	-3.38544	2.010718	-1.39403
C13	-2.08871	1.661397	-1.06245
N14	-1.80984	0.894932	0.016115
H15	2.041995	0.29375	2.006479
H16	2.388162	-0.39698	4.372619
H17	0.383292	-1.25885	5.654609
H18	-1.86208	-1.04928	4.609639
H19	-3.18706	-0.75076	2.525758
H20	-4.89618	0.522372	1.242749
H21	-5.46042	1.727121	-0.85369
H22	-3.56648	2.620067	-2.27244

H23	-1.23784	1.957727	-1.65761
S24	-3.1369	1.448748	3.578976
O25	-4.41572	1.884072	3.030175
O26	-3.26192	0.661942	4.804525
O27	-2.06515	2.428913	3.552906
O28	1.951861	-0.94888	0.096277
C29	2.96117	-0.96973	-0.6182
O30	3.067634	-1.32416	-1.84631
C31	4.330852	-0.77543	0.068886
F32	5.265264	-0.31225	-0.76052
F33	4.24237	0.046402	1.125472
F34	4.745183	-1.98387	0.530598
O35	-0.19861	-0.02034	-2.12879
C36	0.097726	-0.81844	-3.05366
O37	0.975445	-1.70552	-3.10985
C38	-0.81655	-0.68204	-4.30116
F39	-0.21891	-1.12696	-5.41812
F40	-1.94158	-1.41178	-4.11831
F41	-1.18896	0.593716	-4.51192
H42	2.135297	-1.50405	-2.30448
O43	0.892886	2.031613	-0.20753
C44	1.967861	2.262402	-0.84482
O45	2.935231	1.535531	-1.10069
C46	2.00428	3.719347	-1.39128
F47	3.123578	3.988467	-2.08852
F48	0.953489	3.935748	-2.22465
F49	1.920248	4.62996	-0.39699
C50	-0.86999	-1.87126	0.007832
H51	-0.82037	-2.32595	1.001491
H52	-1.91197	-1.81395	-0.3212
H53	-0.29384	-2.4754	-0.69847

Table S161. $Rh^{III}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3^{ax})$

Atom	x	y	z
Rh1	0.151108	-0.21069	-0.00322
N2	0.07523	-0.21151	2.05098
C3	1.170387	-0.46172	2.794972
C4	1.153276	-0.37301	4.17923
C5	-0.03276	-0.00266	4.812335
C6	-1.15572	0.262369	4.037597

C7	-1.08331	0.149297	2.646572
C8	-2.26324	0.481658	1.779888
C9	-2.64799	-0.58011	0.790155
C10	-3.96295	-1.04607	0.709466
C11	-4.30509	-1.99278	-0.24898
C12	-3.3224	-2.45541	-1.12327
C13	-2.03476	-1.9529	-1.00649
N14	-1.70917	-1.04463	-0.06546
H15	2.068269	-0.71422	2.247559
H16	2.057343	-0.58168	4.74009
H17	-0.07994	0.085176	5.893421
H18	-2.08943	0.572087	4.493186
H19	-3.12132	0.686087	2.421601
H20	-4.70546	-0.64725	1.391303
H21	-5.3253	-2.35754	-0.31872
H22	-3.54319	-3.18439	-1.8948
H23	-1.2411	-2.24075	-1.6818
S24	-1.98835	2.13309	0.908498
O25	-3.2202	2.330562	0.17558
O26	-1.69038	3.03595	2.00003
O27	-0.81222	1.852109	0.033624
O28	2.062679	0.681801	0.213413
C29	2.405769	1.851001	-0.05752
O30	1.942473	2.651581	-0.92245
C31	3.606166	2.388239	0.755933
F32	3.732631	3.710793	0.654674
F33	3.456516	2.066955	2.053549
F34	4.736655	1.809319	0.309069
H35	1.197524	2.243961	-1.62775
C36	1.059112	-2.04629	-0.04105
H37	1.00256	-2.42676	-1.06397
H38	2.107867	-1.90571	0.234914
H39	0.570255	-2.7356	0.65359
O40	0.091008	-0.29104	-2.08902
C41	0.093733	0.699868	-2.87649
O42	0.501222	1.863285	-2.70121
C43	-0.44496	0.366152	-4.29068
F44	0.541594	-0.18714	-5.02554
F45	-1.45817	-0.51857	-4.22481
F46	-0.88142	1.457692	-4.92373

Table S162. $[Rh^{III}(DPMS)(TFAH^{eq})_2(CH_3^{ax})]^+$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.031436
C3	1.147687	0	2.742247
C4	1.149131	0.10253	4.125806
C5	-0.06997	0.215899	4.793284
C6	-1.24769	0.214671	4.052349
C7	-1.19421	0.099516	2.662781
C8	-2.45191	0.106611	1.832586
C9	-2.57926	-1.06345	0.891122
C10	-3.72699	-1.85652	0.881224
C11	-3.82256	-2.9225	-0.00801
C12	-2.76132	-3.17577	-0.87598
C13	-1.64715	-2.35019	-0.82889
N14	-1.56237	-1.31844	0.035522
H15	2.065209	-0.07578	2.173598
H16	2.092206	0.0973	4.660578
H17	-0.10342	0.305215	5.87441
H18	-2.21178	0.31164	4.538604
H19	-3.30844	0.09676	2.509155
H20	-4.53757	-1.62511	1.562985
H21	-4.71165	-3.54473	-0.02335
H22	-2.78879	-3.99631	-1.584
H23	-0.80221	-2.49602	-1.48843
S24	-2.68109	1.730787	0.947004
O25	-3.90656	1.576972	0.210388
O26	-2.56215	2.731607	1.975495
O27	-1.47028	1.767684	0.003963
O28	1.618533	1.383399	0.008549
C29	1.530049	2.617339	0.147663
O30	0.470305	3.331181	0.247006
C31	2.833899	3.446739	0.226153
F32	3.900477	2.654849	0.117196
F33	2.84729	4.346466	-0.76406
F34	2.876093	4.083708	1.402259
O35	-0.17306	-0.0316	-2.15473
C36	-0.34739	0.897697	-2.93055
O37	-0.11529	2.150584	-2.63216
C38	-0.86435	0.589246	-4.35928

F39	-1.04408	1.750802	-5.02349
F40	0.026159	-0.1548	-5.00855
F41	-2.02444	-0.05618	-4.2822
H42	-0.40447	2.76868	0.188488
H43	-0.35531	2.739509	-3.37176
C50	1.376617	-1.5144	-0.07458
H51	2.35515	-1.07077	0.123093
H52	1.138684	-2.28704	0.659534
H53	1.361402	-1.92484	-1.08747

Table S163. $Rh^{III}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3^{eq})$

Atom	x	y	z
Rh1	0.023077	-0.13638	0.095069
N2	-0.57214	-0.74914	2.205068
C3	0.267939	-1.25777	3.114335
C4	-0.08741	-1.4188	4.449788
C5	-1.36349	-1.02243	4.846883
C6	-2.23746	-0.49691	3.898086
C7	-1.8106	-0.37838	2.573406
C8	-2.72003	0.178357	1.498332
C9	-2.85377	-0.7093	0.286738
C10	-4.08126	-1.28178	-0.05057
C11	-4.18377	-2.09651	-1.17267
C12	-3.04467	-2.33284	-1.93905
C13	-1.8499	-1.73763	-1.56009
N14	-1.7618	-0.93815	-0.47929
H15	1.251189	-1.53717	2.748809
H16	0.622021	-1.83817	5.154985
H17	-1.67579	-1.12232	5.882062
H18	-3.23498	-0.17409	4.175928
H19	-3.71408	0.330212	1.923232
H20	-4.94606	-1.07718	0.570423
H21	-5.13643	-2.54204	-1.44182
H22	-3.06961	-2.96693	-2.81809
H23	-0.93187	-1.90655	-2.10473
S24	-2.23036	1.890896	0.97294
O25	-3.10461	2.179076	-0.14167
O26	-2.33384	2.702129	2.161722
O27	-0.78143	1.717902	0.55592
O28	1.769264	0.776394	0.918287

C29	2.884211	1.081844	0.483195
O30	3.52418	0.583891	-0.51185
C31	3.668354	2.205401	1.199639
F32	3.898551	3.209165	0.339725
F33	2.990361	2.675751	2.245644
F34	4.850422	1.730286	1.62948
C35	0.377426	0.57535	-1.80232
H36	0.771418	-0.212	-2.45104
H37	-0.56845	0.960279	-2.18935
H38	1.095077	1.396317	-1.73658
H39	3.100664	-0.31009	-0.88146
O40	0.799932	-2.01795	-0.30253
C41	1.850504	-2.33418	-0.93856
O42	2.812759	-1.63979	-1.30602
C43	1.862314	-3.8338	-1.33136
F44	0.87432	-4.05888	-2.22956
F45	3.019494	-4.20249	-1.88414
F46	1.632855	-4.6135	-0.26058

Table S164. $[Rh^{IV}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq})]^+$

Atom	x	y	z
Rh1	0.01108	-0.11686	0.058626
N2	-0.56824	-0.76184	2.17837
C3	0.274538	-1.314	3.061216
C4	-0.09065	-1.54895	4.383944
C5	-1.37124	-1.18586	4.795754
C6	-2.24613	-0.61031	3.873355
C7	-1.80991	-0.41582	2.56468
C8	-2.71577	0.193146	1.507739
C9	-2.88322	-0.67047	0.278428
C10	-4.12149	-1.21637	-0.05253
C11	-4.23938	-2.04043	-1.16956
C12	-3.10545	-2.31128	-1.93178
C13	-1.89659	-1.73773	-1.56244
N14	-1.79733	-0.92718	-0.48972
H15	1.261666	-1.56964	2.690541
H16	0.617591	-2.00139	5.069187
H17	-1.68817	-1.34714	5.821263
H18	-3.24695	-0.31224	4.166841
H19	-3.70168	0.368926	1.944773

H20	-4.98325	-0.9919	0.566097
H21	-5.20111	-2.46756	-1.43513
H22	-3.14413	-2.95608	-2.8024
H23	-0.98495	-1.9375	-2.10785
S24	-2.18927	1.888237	1.037359
O25	-3.05999	2.33096	-0.0142
O26	-2.02393	2.636461	2.248219
O27	-0.75547	1.647671	0.419756
O28	1.760418	0.776855	0.861111
C29	2.883091	1.12901	0.458553
O30	3.555911	0.648742	-0.51839
C31	3.555408	2.301248	1.217357
F32	2.871689	3.419132	0.944336
F33	3.49622	2.05693	2.530844
F34	4.822621	2.453008	0.848871
C35	0.416533	0.523465	-1.88038
H36	0.900395	-0.28116	-2.43298
H37	-0.54108	0.802775	-2.31942
H38	1.067975	1.392125	-1.7889
H39	3.148275	-0.22357	-0.88926
O40	0.748632	-1.95912	-0.28249
C41	1.831625	-2.31004	-0.89383
O42	2.773754	-1.6154	-1.26898
C43	1.830428	-3.82833	-1.21482
F44	0.830918	-4.06617	-2.09213
F45	2.979945	-4.2105	-1.75421
F46	1.599644	-4.53789	-0.10271

Table S165. $[Rh^{IV}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3^{ax})]^+$

Atom	x	y	z
Rh1	0.101184	-0.14155	-0.03294
N2	0.060013	-0.18413	2.055849
C3	1.170262	-0.41641	2.784134
C4	1.144919	-0.41421	4.172683
C5	-0.05878	-0.15379	4.824554
C6	-1.19497	0.11424	4.064054
C7	-1.11037	0.097714	2.673719
C8	-2.29553	0.462598	1.811512
C9	-2.6899	-0.58859	0.80295
C10	-3.99028	-1.0852	0.74998

C11	-4.32498	-2.03996	-0.20869
C12	-3.34886	-2.4711	-1.10416
C13	-2.07088	-1.93513	-1.01447
N14	-1.75358	-1.0246	-0.07197
H15	2.084707	-0.58347	2.231454
H16	2.05872	-0.60845	4.722756
H17	-0.11139	-0.14422	5.908579
H18	-2.14011	0.351506	4.539642
H19	-3.15147	0.663021	2.459116
H20	-4.73193	-0.71445	1.448784
H21	-5.33557	-2.43261	-0.25922
H22	-3.56571	-3.2038	-1.87318
H23	-1.2873	-2.20274	-1.71023
S24	-1.98891	2.103612	1.008676
O25	-3.15622	2.413489	0.222738
O26	-1.58328	2.979117	2.077556
O27	-0.81227	1.818468	0.075183
O28	2.011647	0.739142	0.15579
C29	2.393728	1.905054	-0.09333
O30	1.914872	2.740871	-0.91952
C31	3.643559	2.388747	0.683613
F32	3.698587	3.714202	0.729405
F33	3.598591	1.903782	1.935593
F34	4.736103	1.911596	0.07447
H35	1.182822	2.35598	-1.58388
C36	1.078674	-1.95267	0.002106
H37	1.010801	-2.31647	-1.0249
H38	2.117919	-1.74966	0.260422
H39	0.593144	-2.6219	0.712114
O40	0.038401	-0.26549	-2.06783
C41	0.088667	0.719174	-2.89158
O42	0.42361	1.887663	-2.68134
C43	-0.35164	0.305667	-4.32029
F44	0.532151	-0.57488	-4.81578
F45	-1.55742	-0.29101	-4.25748
F46	-0.42759	1.356299	-5.12676

Table S166. $Rh^{IV}(DPMS)(TFA)_2(CH_3^{eq})$

Atom	x	y	z
Rh1	-0.04559	-0.04919	-0.06753

N2	-0.61885	-0.56442	2.131039
C3	0.266889	-0.98076	3.043412
C4	-0.07697	-1.13761	4.383623
C5	-1.37843	-0.83198	4.776986
C6	-2.29047	-0.37949	3.824355
C7	-1.87136	-0.25693	2.499154
C8	-2.8008	0.258106	1.415382
C9	-2.96777	-0.6792	0.241893
C10	-4.19038	-1.30401	-0.00906
C11	-4.31356	-2.17223	-1.08967
C12	-3.20534	-2.40152	-1.90222
C13	-2.01608	-1.75005	-1.60516
N14	-1.90665	-0.90761	-0.56222
H15	1.271829	-1.16718	2.67863
H16	0.663991	-1.48145	5.096989
H17	-1.68	-0.93531	5.814998
H18	-3.30455	-0.11338	4.103367
H19	-3.78529	0.437355	1.853354
H20	-5.03333	-1.10315	0.642902
H21	-5.26021	-2.66371	-1.29191
H22	-3.25061	-3.07363	-2.75166
H23	-1.11701	-1.90674	-2.18647
S24	-2.31683	1.943763	0.832582
O25	-3.24952	2.261918	-0.2193
O26	-2.25627	2.767689	2.010302
O27	-0.90008	1.746498	0.255441
O28	1.684823	0.530372	0.743791
C29	2.584649	1.388517	0.337635
O30	2.548759	2.183368	-0.57605
C31	3.809956	1.331322	1.291498
F32	3.490245	1.882626	2.482829
F33	4.194591	0.059581	1.521625
F34	4.84957	2.000443	0.786716
C35	0.284256	0.606079	-2.00925
H36	0.693065	-0.22946	-2.5767
H37	-0.69312	0.925414	-2.37321
H38	0.992867	1.424478	-1.92107
O39	0.691744	-1.84737	-0.44971
C40	1.908243	-2.073	-0.90558
O41	2.742628	-1.28396	-1.28459

C42	2.173308	-3.60119	-0.92661
F43	1.258725	-4.21776	-1.70753
F44	3.387222	-3.87569	-1.40568
F45	2.075469	-4.11908	0.313378

Table S167. $Rh^{IV}(DPMS)(TFA)_2(CH_3^{ax})$

Atom	x	y	z
Rh1	0.156123	-0.20587	0.021304
N2	0.064268	-0.2253	2.066933
C3	1.15948	-0.47139	2.812323
C4	1.135961	-0.39596	4.197224
C5	-0.05598	-0.04231	4.828826
C6	-1.17803	0.220006	4.052089
C7	-1.1004	0.120109	2.660332
C8	-2.28127	0.447143	1.792959
C9	-2.65156	-0.61287	0.796725
C10	-3.96069	-1.09372	0.707837
C11	-4.28609	-2.04186	-0.25453
C12	-3.29238	-2.49263	-1.12293
C13	-2.01182	-1.97472	-0.99662
N14	-1.70244	-1.06217	-0.05478
H15	2.061327	-0.70998	2.264914
H16	2.039578	-0.60209	4.75984
H17	-0.10839	0.034466	5.910519
H18	-2.11607	0.516811	4.50719
H19	-3.14244	0.640156	2.433896
H20	-4.71135	-0.70628	1.387194
H21	-5.30128	-2.41909	-0.33064
H22	-3.49955	-3.22555	-1.89457
H23	-1.20772	-2.2619	-1.66045
S24	-2.02002	2.104056	0.925495
O25	-3.25547	2.291275	0.194789
O26	-1.73278	3.005962	2.02072
O27	-0.84343	1.836457	0.048839
O28	2.052377	0.663591	0.230004
C29	2.401862	1.804685	-0.16438
O30	1.991388	2.535798	-1.08978
C31	3.601296	2.395222	0.646587
F32	3.893782	3.645588	0.292433
F33	3.302855	2.37431	1.956391

F34	4.684892	1.623803	0.449036
C35	1.075525	-2.03806	-0.02154
H36	1.031619	-2.41337	-1.04734
H37	2.121172	-1.89711	0.264653
H38	0.582091	-2.73492	0.662355
O39	0.132275	-0.24598	-2.07332
C40	0.188517	0.743331	-2.84596
O41	0.669977	1.888167	-2.71279
C42	-0.44331	0.463182	-4.24841
F43	0.259603	-0.50663	-4.85956
F44	-1.7046	0.030149	-4.08548
F45	-0.45654	1.541623	-5.03037

Table S168. Rh^{II}(DPMS)(TFA)(TFAH)

Atom	x	y	z
Rh1	-0.00611	-0.00674	-0.00075
N2	0.007183	-0.00278	2.065494
C3	1.164796	0.003731	2.756135
C4	1.193017	0.096243	4.140446
C5	-0.01618	0.202779	4.827988
C6	-1.20506	0.20394	4.107926
C7	-1.17347	0.09292	2.715487
C8	-2.43543	0.127086	1.90039
C9	-2.60384	-1.02343	0.946931
C10	-3.76422	-1.80218	0.95129
C11	-3.90508	-2.83921	0.036044
C12	-2.88256	-3.07601	-0.88265
C13	-1.75881	-2.26265	-0.85299
N14	-1.62446	-1.26949	0.048665
H15	2.070667	-0.04067	2.163984
H16	2.145317	0.096419	4.659072
H17	-0.0313	0.289712	5.910083
H18	-2.16121	0.304015	4.608633
H19	-3.28869	0.140933	2.579894
H20	-4.54879	-1.57713	1.664863
H21	-4.80333	-3.44925	0.033862
H22	-2.9526	-3.86658	-1.62146
H23	-0.95533	-2.36086	-1.57239
S24	-2.60131	1.780299	1.007443
O25	-3.8639	1.653472	0.311781

O26	-2.50906	2.742283	2.08561
O27	-1.41676	1.803585	0.095013
O28	1.710118	1.244703	0.111183
C29	1.78385	2.452007	-0.19551
O30	1.130813	3.101986	-1.06672
C31	2.8522	3.268399	0.567557
F32	2.691527	4.581497	0.410222
F33	2.791182	2.979673	1.879874
F34	4.074391	2.924498	0.119353
O35	-0.04824	-0.23185	-2.07565
C36	-0.2454	0.693767	-2.91579
O37	-0.12	1.926444	-2.78522
C38	-0.67011	0.213901	-4.32714
F39	0.375572	0.309936	-5.17142
F40	-1.07824	-1.0678	-4.31608
F41	-1.66913	0.967198	-4.80349
H42	0.489709	2.511807	-1.73382

Table S169. [Rh^{III}(DPMS)(TFA^{eq})(CH_3^{ax}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.084755
C3	1.146582	0	2.786288
C4	1.159045	-0.00148	4.174134
C5	-0.05893	0.006991	4.852467
C6	-1.24076	0.027362	4.118952
C7	-1.18722	0.026816	2.724046
C8	-2.43012	0.122828	1.882185
C9	-2.63554	-1.00295	0.904683
C10	-3.82073	-1.73929	0.883126
C11	-4.00214	-2.72298	-0.08418
C12	-2.99779	-2.94217	-1.02478
C13	-1.84189	-2.17491	-0.96056
N14	-1.66545	-1.24507	-0.00441
H15	2.061072	0.010045	2.207004
H16	2.105608	-0.00378	4.702711
H17	-0.08761	0.007304	5.937705
H18	-2.20479	0.057376	4.614181
H19	-3.29928	0.186546	2.53862
H20	-4.59318	-1.52261	1.612347
H21	-4.92138	-3.29984	-0.11125

H22	-3.10492	-3.68213	-1.80977
H23	-1.04933	-2.25361	-1.69362
S24	-2.44361	1.767216	0.983561
O25	-3.75376	1.846844	0.384853
O26	-2.08243	2.725564	2.000174
O27	-1.36532	1.575512	-0.06837
O28	1.493654	1.431892	0.074119
C29	2.538244	1.137664	-0.5757
O30	2.848637	-0.00846	-0.97822
C31	3.56062	2.276358	-0.76617
F32	4.302673	2.081228	-1.85775
F33	2.970829	3.467211	-0.84072
F34	4.38313	2.274355	0.311786
O35	-0.14771	-0.17176	-2.0258
C36	0.299117	0.667224	-2.91474
O37	1.054898	1.611727	-2.80068
C38	-0.29065	0.294713	-4.30381
F39	0.2534	1.02402	-5.28173
F40	-0.0693	-1.01193	-4.58307
F41	-1.62465	0.491113	-4.32159
H42	1.853103	-0.79897	-0.4862
C43	1.330283	-1.91457	-0.00333
H44	2.262377	-2.08641	0.546619
H45	0.535616	-2.3234	0.617429
H46	1.346636	-2.45888	-0.95101

Table S170. [Rh^{III}(DPMS)(TFAH^{eq})(CH_3^{ax}-H-TFA^{eq})]$^{+‡}$

Atom	x	y	z
Rh1	0	0	0
N2	0	0	2.047116
C3	1.147695	0	2.75671
C4	1.148206	0.071289	4.142437
C5	-0.07068	0.152354	4.812775
C6	-1.24916	0.153301	4.071695
C7	-1.19346	0.07336	2.680961
C8	-2.4488	0.092704	1.846939
C9	-2.60791	-1.07638	0.9085
C10	-3.76832	-1.84957	0.907571
C11	-3.9092	-2.87905	-0.01905
C12	-2.88521	-3.10771	-0.93666
C13	-1.75266	-2.30638	-0.88893
N14	-1.6153	-1.32236	0.022586

H15	2.070929	-0.06006	2.195142
H16	2.092586	0.067137	4.674651
H17	-0.10459	0.21607	5.895555
H18	-2.21406	0.225071	4.560783
H19	-3.31082	0.126764	2.515847
H20	-4.55536	-1.62958	1.620118
H21	-4.80916	-3.48543	-0.03074
H22	-2.95642	-3.88806	-1.68576
H23	-0.93966	-2.43131	-1.59216
S24	-2.59668	1.689281	0.916271
O25	-3.81512	1.606133	0.158921
O26	-2.3913	2.727609	1.883045
O27	-1.374	1.580685	-0.04784
O28	1.346058	1.567089	-0.10395
C29	2.581337	1.293369	-0.08101
O30	3.061266	0.140472	0.02803
C31	3.548002	2.502381	-0.10668
F32	4.714612	2.155889	-0.6466
F33	3.021847	3.515044	-0.79509
F34	3.747344	2.889746	1.165412
O35	0.021706	-0.03374	-2.1133
C36	-0.49529	0.801353	-2.88128
O37	-1.24068	1.797936	-2.57616
C38	-0.20413	0.627198	-4.39125
F39	-0.91994	1.469831	-5.124
F40	1.10022	0.845006	-4.59513
F41	-0.49868	-0.63315	-4.73855
H42	1.989045	-0.72577	0.006397
H43	-1.40407	1.851387	-1.56967
C50	1.334127	-1.86667	-0.10578
H51	2.341022	-2.18297	0.207142
H52	0.66647	-2.40492	0.563043
H53	1.212884	-2.15638	-1.14783

Table S171. [Rh^{III}(DPMS)(TFA^{eq})(CH_3^{eq}-H-TFA^{ax})]‡

Atom	x	y	z
Rh1	-0.13075	-0.1052	-0.06317
N2	-0.12758	-0.0627	2.046812
C3	1.022578	-0.15814	2.72912
C4	1.062281	-0.00417	4.110038
C5	-0.12395	0.273748	4.78597
C6	-1.31115	0.377671	4.064269

C7	-1.28713	0.198363	2.681299
C8	-2.53304	0.304317	1.836099
C9	-2.79404	-0.92153	0.998535
C10	-3.95177	-1.68416	1.162279
C11	-4.15073	-2.81296	0.37421
C12	-3.18053	-3.16101	-0.56408
C13	-2.05423	-2.35857	-0.68403
N14	-1.87124	-1.26217	0.073667
H15	1.910179	-0.3367	2.135315
H16	2.008497	-0.089	4.632564
H17	-0.12588	0.412615	5.862723
H18	-2.2489	0.605377	4.558799
H19	-3.39268	0.479577	2.485195
H20	-4.68569	-1.38347	1.901677
H21	-5.04763	-3.41315	0.492384
H22	-3.28746	-4.03502	-1.19669
H23	-1.27195	-2.58367	-1.39739
S24	-2.49297	1.818689	0.753269
O25	-3.59925	1.633776	-0.15667
O26	-2.51465	2.937507	1.661789
O27	-1.13864	1.704849	0.067883
O28	1.639586	0.890973	0.072704
C29	1.989581	1.881262	-0.70041
O30	1.484352	2.289606	-1.72504
C31	3.270548	2.552359	-0.13336
F32	3.060415	3.010298	1.119208
F33	4.288026	1.662697	-0.07553
F34	3.662364	3.580352	-0.8918
H35	0.286454	0.443418	-3.04757
H36	0.772853	-0.58255	-1.96591
O37	1.023205	-1.83633	0.020432
C38	1.788288	-2.01095	-0.96685
O39	1.760367	-1.36837	-2.04599
C40	2.807738	-3.16345	-0.85791
F41	3.946307	-2.85113	-1.48075
F42	3.076966	-3.44897	0.421318
F43	2.283417	-4.26036	-1.43874
C44	-0.41636	0.078776	-2.28833
H45	-1.04185	-0.71749	-2.70023
H46	-1.01568	0.96016	-2.06839

Table S172. [Rh^{III}(DPMS)(TFA^{ax})(CH_3^{eq}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	-0.03167	-0.15505	-0.18198
N2	-0.01656	-0.13044	1.908576
C3	1.118789	-0.31636	2.598617
C4	1.167211	-0.13091	3.975436
C5	0.007416	0.266387	4.638217
C6	-1.16766	0.443039	3.911007
C7	-1.15785	0.228523	2.533
C8	-2.40538	0.365713	1.690946
C9	-2.69335	-0.88374	0.897276
C10	-3.86266	-1.61997	1.091089
C11	-4.05576	-2.80302	0.38441
C12	-3.06221	-3.23728	-0.49077
C13	-1.92467	-2.45712	-0.64961
N14	-1.76223	-1.29675	0.010833
H15	1.984419	-0.60782	2.017408
H16	2.099449	-0.28827	4.506031
H17	0.014492	0.432901	5.711036
H18	-2.08721	0.749049	4.397469
H19	-3.2548	0.573791	2.343784
H20	-4.606	-1.26129	1.794285
H21	-4.96144	-3.38459	0.526784
H22	-3.15514	-4.16582	-1.04268
H23	-1.10697	-2.75954	-1.28908
S24	-2.34211	1.855241	0.578082
O25	-3.45113	1.666854	-0.32873
O26	-2.35175	2.992633	1.464327
O27	-0.99309	1.698816	-0.0975
O28	1.736787	0.915663	-0.03569
C29	2.097223	1.553005	-1.06509
O30	1.517905	1.555534	-2.17145
C31	3.364963	2.413628	-0.88829
F32	3.114156	3.402702	-0.01251
F33	4.366804	1.662855	-0.40197
F34	3.756679	2.955273	-2.0432
H35	-0.10925	0.269715	-3.36022
H36	0.56288	0.657737	-2.09159
O37	0.966034	-1.9274	-0.15398
C38	1.983985	-2.1408	-0.939
O39	2.485901	-1.41939	-1.77889
C40	2.540126	-3.56846	-0.69024

F41	3.587345	-3.83267	-1.47571
F42	2.928002	-3.71765	0.593925
F43	1.583745	-4.49252	-0.94126
C44	-0.42249	-0.22664	-2.42966
H45	-0.21021	-1.28086	-2.59298
H46	-1.48521	-0.009	-2.3352

Table S173. [Rh^{III}(DPMS)($TFAH^{eq}$)(CH_3^{eq}-H-TFA^{ax})]$^{+‡}$

Atom	x	y	z
Rh1	-0.13037	-0.19291	-0.12467
N2	-0.10105	-0.09643	1.969902
C3	1.044509	-0.2638	2.653505
C4	1.089428	-0.12402	4.035289
C5	-0.08403	0.197663	4.715437
C6	-1.26849	0.352776	3.996264
C7	-1.25165	0.192194	2.612342
C8	-2.49897	0.322856	1.769947
C9	-2.77921	-0.897	0.922749
C10	-3.97637	-1.60138	1.040158
C11	-4.18801	-2.74006	0.266628
C12	-3.18878	-3.1587	-0.61008
C13	-2.02095	-2.41404	-0.69631
N14	-1.83129	-1.30577	0.046294
H15	1.919512	-0.52144	2.068846
H16	2.028661	-0.26536	4.558029
H17	-0.08062	0.321245	5.793749
H18	-2.19756	0.600367	4.497792
H19	-3.35459	0.496574	2.425933
H20	-4.73266	-1.25173	1.734035
H21	-5.11755	-3.29382	0.35161
H22	-3.30432	-4.04404	-1.22492
H23	-1.21825	-2.6919	-1.36614
S24	-2.46356	1.856846	0.744562
O25	-3.6602	1.833454	-0.04534
O26	-2.17761	2.94389	1.638978
O27	-1.2099	1.598301	-0.16194
O28	1.679229	0.897518	-0.23837
C29	1.823836	2.132938	-0.27887
O30	0.904974	3.03007	-0.27166
C31	3.266152	2.694701	-0.28325
F32	3.620393	2.91282	0.993308
F33	4.098022	1.805052	-0.82374

F34	3.323286	3.836	-0.96148
H35	0.325254	0.409302	-3.08556
H42	0.687453	-0.81904	-2.00621
O50	1.05028	-1.85985	0.074654
C51	1.781958	-2.15313	-0.92428
O52	1.692403	-1.64272	-2.06101
C53	2.849053	-3.23917	-0.65635
F54	3.624269	-3.42038	-1.71795
F55	3.600546	-2.85479	0.385974
F56	2.232738	-4.38935	-0.35018
C49	-0.38202	-0.08732	-2.4091
H50	-0.88304	-0.90753	-2.93034
H51	-1.13214	0.66507	-2.1692
H47	-0.02235	2.613771	-0.20514

Table S174. [$Rh^{III\text{-}I}$(DPMS)(TFA^{eq})($TFAH^{eq}$)(CH_3^{ax}-TFA)]$^{-‡}$

Atom	x	y	z
Rh1	0.230233	-0.34841	-0.15691
N2	0.165029	-0.20803	1.886297
C3	1.288545	-0.3477	2.626776
C4	1.305025	-0.13316	3.996895
C5	0.123136	0.249412	4.63145
C6	-1.03224	0.372466	3.872164
C7	-0.99768	0.123458	2.494367
C8	-2.25123	0.265243	1.685915
C9	-2.54481	-0.82445	0.698724
C10	-3.84817	-1.33194	0.606561
C11	-4.15168	-2.32231	-0.3163
C12	-3.13735	-2.7944	-1.15066
C13	-1.87053	-2.24512	-1.03273
N14	-1.57551	-1.28238	-0.13078
H15	2.183583	-0.65465	2.101035
H16	2.232526	-0.26736	4.542649
H17	0.101563	0.442744	5.700338
H18	-1.96935	0.679418	4.322366
H19	-3.08884	0.304891	2.384205
H20	-4.61298	-0.91834	1.253824
H21	-5.16173	-2.71543	-0.38939
H22	-3.31942	-3.56527	-1.89193
H23	-1.05909	-2.53567	-1.68652
S24	-2.37639	1.997348	0.898499
O25	-3.70149	1.949071	0.293037

O26	-2.24468	2.852059	2.072503
O27	-1.26014	2.061825	-0.04632
O28	2.038046	0.829471	-0.03879
C29	2.186779	2.007403	-0.38977
O30	1.599162	2.665307	-1.31372
C31	3.280191	2.821082	0.338696
F32	4.457173	2.672573	-0.30898
F33	2.990135	4.12812	0.377346
F34	3.442788	2.387096	1.596763
O35	0.213769	-0.62307	-2.26188
C36	0.084176	0.290331	-3.11939
O37	0.291711	1.518056	-3.03264
C38	-0.38091	-0.23426	-4.50133
F39	-0.68504	0.753379	-5.35443
F40	0.592269	-0.98387	-5.06774
F41	-1.4719	-1.0201	-4.37392
H42	0.937005	2.095901	-1.94888
C43	1.77205	-2.33962	-0.08594
H44	2.504384	-1.55552	0.003295
H45	1.236526	-2.67013	0.788167
H46	1.433891	-2.63683	-1.06643
O47	3.039725	-3.70702	-0.002
C48	3.825173	-3.55255	1.003495
O49	3.82771	-2.69438	1.880812
C50	4.919213	-4.65943	1.034655
F51	4.369819	-5.89517	1.067163
F52	5.705892	-4.59754	-0.06349
F53	5.719067	-4.5473	2.11008

Table S175. $[Rh^{III\text{-}II}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{\ddagger}$

Atom	x	y	z
Rh1	0.382671	-0.05249	-0.21989
N2	0.363188	0.108185	1.843755
C3	1.495469	0.096107	2.574493
C4	1.484418	0.296095	3.948065
C5	0.266133	0.534827	4.581117
C6	-0.89741	0.556239	3.819199
C7	-0.82781	0.3332	2.443327
C8	-2.06139	0.374436	1.583423
C9	-2.27447	-0.85308	0.740464
C10	-3.46596	-1.57796	0.803135
C11	-3.64582	-2.6856	-0.01809

C12	-2.63116	-3.04202	-0.90495
C13	-1.47261	-2.2798	-0.9343
N14	-1.29695	-1.22198	-0.11768
H15	2.419538	-0.06769	2.036476
H16	2.418134	0.266966	4.497736
H17	0.222158	0.704554	5.652423
H18	-1.86101	0.753632	4.275158
H19	-2.93221	0.509739	2.226691
H20	-4.24309	-1.25878	1.488258
H21	-4.56759	-3.25708	0.027287
H22	-2.7294	-3.89019	-1.57281
H23	-0.67106	-2.48463	-1.63096
S24	-2.08661	1.921383	0.524996
O25	-3.29638	1.78934	-0.25378
O26	-1.98908	2.999632	1.482002
O27	-0.83467	1.781583	-0.30616
O28	2.135052	1.140716	-0.15473
C29	2.280147	2.325379	-0.52277
O30	1.677796	2.961124	-1.4394
C31	3.37326	3.121106	0.227144
F32	4.579064	2.627704	-0.10279
F33	3.340568	4.419402	-0.06615
F34	3.202756	2.970257	1.55227
O35	0.313091	-0.37072	-2.27366
C36	0.186212	0.519934	-3.17133
O37	0.393439	1.742079	-3.1136
C38	-0.26255	-0.07064	-4.53109
F39	-0.5792	0.879415	-5.41029
F40	0.735467	-0.81793	-5.04415
F41	-1.33317	-0.87056	-4.35933
H42	1.021404	2.372443	-2.07355
C43	1.873112	-1.94056	-0.2968
H44	2.671176	-1.27767	0.006936
H45	1.268249	-2.45145	0.439297
H46	1.680961	-2.07295	-1.35118
O47	3.147238	-3.45402	-0.34854
V48	3.720777	-4.03226	1.074389
Cl49	5.150976	-5.64153	0.859162
Cl50	4.61936	-2.31354	2.116806
Cl51	1.957943	-4.67899	2.221547

Table S176. $[Rh^{IV\text{-}II}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{\ddagger}$

Atom	x	y	z
Rh1	0.197494	-0.26511	-0.19481
N2	0.187542	-0.18004	1.866866
C3	1.314247	-0.34294	2.589255
C4	1.320829	-0.1818	3.968893
C5	0.136507	0.168276	4.612661
C6	-1.02227	0.325883	3.857892
C7	-0.9762	0.138498	2.476694
C8	-2.20317	0.304497	1.621809
C9	-2.5114	-0.87674	0.741458
C10	-3.7574	-1.50538	0.782079
C11	-4.02673	-2.56455	-0.07779
C12	-3.04496	-2.96974	-0.98041
C13	-1.82663	-2.30594	-0.98453
N14	-1.56665	-1.29616	-0.13109
H15	2.211325	-0.62694	2.054318
H16	2.246579	-0.331	4.512657
H17	0.112286	0.312786	5.688331
H18	-1.96143	0.600999	4.324359
H19	-3.06052	0.48806	2.271229
H20	-4.50586	-1.14885	1.480568
H21	-4.99199	-3.0604	-0.04981
H22	-3.21311	-3.78098	-1.67953
H23	-1.04064	-2.55077	-1.68614
S24	-2.10909	1.872964	0.603655
O25	-3.35578	1.892758	-0.12561
O26	-1.85577	2.910896	1.576291
O27	-0.91684	1.617072	-0.2867
O28	2.005907	0.834868	-0.07427
C29	2.204227	2.030983	-0.37258
O30	1.660606	2.733632	-1.27761
C31	3.28859	2.751831	0.461413
F32	3.310683	4.063264	0.228029
F33	3.052501	2.547961	1.768863
F34	4.492018	2.234844	0.162306
O35	0.107483	-0.50169	-2.25953
C36	0.086877	0.421593	-3.13163
O37	0.39322	1.620648	-3.0356
C38	-0.42637	-0.07079	-4.50848
F39	-0.1773	0.810063	-5.47883
F40	0.14916	-1.24266	-4.83692

F41	-1.75847	-0.26874	-4.43925
H42	1.008846	2.194545	-1.9569
C43	1.353051	-2.17076	-0.19532
H44	2.246499	-1.6414	0.121625
H45	0.798716	-2.74435	0.536453
H46	1.284036	-2.47677	-1.23168
O47	2.796507	-3.78961	0.084839
C48	3.567489	-3.47744	1.062197
O49	3.620378	-2.46643	1.751439
C50	4.60955	-4.6249	1.332155
F51	4.030814	-5.83651	1.307057
F52	5.568168	-4.59327	0.389721
F53	5.18727	-4.46142	2.527254

Table S177. $[Rh^{IV\text{-}II}(DPMS)(TFA)_2(CH_3^{ax}\text{-}TFA)]^{\cdot\ddagger}$

Atom	x	y	z
Rh1	-0.00898	-0.07673	-0.16752
N2	0.137341	-0.23654	1.900531
C3	1.3288	-0.38556	2.510923
C4	1.438167	-0.46417	3.894539
C5	0.287324	-0.36433	4.667503
C6	-0.94034	-0.20941	4.029331
C7	-0.99464	-0.16023	2.63655
C8	-2.31098	-0.02252	1.923976
C9	-2.5849	-1.11061	0.923319
C10	-3.76852	-1.85	0.993822
C11	-4.03046	-2.82982	0.043967
C12	-3.09788	-3.04695	-0.9669
C13	-1.93952	-2.27895	-0.99398
N14	-1.68831	-1.33403	-0.06503
H15	2.199699	-0.44925	1.872866
H16	2.417324	-0.61632	4.332849
H17	0.338716	-0.41404	5.751499
H18	-1.86096	-0.12571	4.596417
H19	-3.10809	-0.03019	2.669236
H20	-4.47513	-1.6356	1.787977
H21	-4.94968	-3.40724	0.089912
H22	-3.25662	-3.79146	-1.73938
H23	-1.20275	-2.37795	-1.78591
S24	-2.49935	1.654593	1.121168
O25	-3.85841	1.635338	0.613318
O26	-2.20681	2.589186	2.190404

O27	-1.46442	1.619857	0.046776
O28	1.442232	1.377023	-0.26721
C29	2.703773	1.266881	-0.08804
O30	3.383865	0.293961	0.239599
C31	3.445853	2.603034	-0.3742
F32	3.760203	2.682653	-1.686
F33	2.71277	3.684156	-0.05953
F34	4.596491	2.673828	0.324095
O35	-0.17811	0.301866	-2.19776
C36	-0.15836	-0.45806	-3.22276
O37	-0.10008	-1.68594	-3.32307
C38	-0.18567	0.358186	-4.54798
F39	-0.8644	-0.30687	-5.50752
F40	-0.75237	1.568589	-4.41771
F41	1.077512	0.540087	-4.99837
C43	1.211322	-1.87079	-0.38093
H44	2.110384	-1.25504	-0.22545
H45	0.903965	-2.51299	0.436365
H46	1.063337	-2.25361	-1.38468
O47	3.249196	-3.05427	-0.1934
C48	3.538992	-3.17098	1.042398
O49	2.916774	-2.88169	2.061437
C50	4.934805	-3.86115	1.25417
F51	5.785907	-3.68765	0.228296
F52	5.533776	-3.39318	2.365489
F53	4.761532	-5.19539	1.420314

Table S178. $[Rh^{III}(DPMS)(TFA^{eq})(CH_2TFA^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	-0.26446	-0.04068	0.001671
N2	-0.11431	0.07131	2.102006
C3	1.063968	0.004333	2.751612
C4	1.148321	0.063055	4.136175
C5	-0.02604	0.200527	4.873546
C6	-1.23875	0.279091	4.197261
C7	-1.25904	0.213975	2.803281
C8	-2.5408	0.354295	2.029686
C9	-2.88431	-0.81261	1.142886
C10	-4.12495	-1.44356	1.230547
C11	-4.43908	-2.47051	0.345107
C12	-3.50735	-2.83726	-0.62249
C13	-2.28888	-2.17109	-0.67043

N14	-1.98401	-1.19838	0.209791
H15	1.950734	-0.10162	2.137876
H16	2.119133	0.004187	4.615295
H17	0.002308	0.251611	5.957574
H18	-2.17126	0.40254	4.736476
H19	-3.36055	0.520836	2.730154
H20	-4.83672	-1.1121	1.978157
H21	-5.40304	-2.96651	0.402903
H22	-3.71422	-3.61764	-1.34598
H23	-1.5433	-2.38894	-1.42262
S24	-2.48891	1.936808	1.034854
O25	-3.83897	2.137591	0.57158
O26	-1.90554	2.90206	1.934509
O27	-1.57321	1.557531	-0.12123
O28	1.215675	1.385728	-0.27545
C29	2.408573	0.986115	-0.26816
O30	2.789525	-0.18967	-0.03551
C31	3.496715	2.064658	-0.45806
F32	4.581648	1.552442	-1.04364
F33	3.05118	3.091294	-1.18223
F34	3.847841	2.521187	0.76499
O35	-0.63182	-0.19025	-1.98664
C36	0.31021	-0.27998	-2.8728
O37	1.519956	-0.28202	-2.72476
C38	-0.31871	-0.46146	-4.28188
F39	0.618766	-0.53866	-5.2306
F40	-1.0392	-1.61013	-4.31065
F41	-1.14773	0.551144	-4.58565
H42	1.669956	-0.94074	-0.04377
C43	0.953156	-2.07595	0.089483
H44	1.918009	-2.43405	0.476146
H45	0.20186	-2.3965	0.807632
O46	0.685982	-2.7419	-1.15038
C47	1.698073	-3.4038	-1.73443
O48	2.799929	-3.57595	-1.28634
C49	1.248962	-3.94477	-3.11132
F50	1.515886	-3.04767	-4.0683
F51	1.909972	-5.07413	-3.38368
F52	-0.07222	-4.20878	-3.12921

Table S179. [Rh^{III}(DPMS)(TFA^{eq})(CH_2TFA^{eq}-H-TFA^{ax})]‡

Atom	x	y	z

Rh1	-0.56015	-0.222	-0.18066
N2	-0.4062	0.061567	1.881728
C3	0.769203	0.379157	2.446945
C4	0.85979	0.691754	3.798167
C5	-0.30253	0.692464	4.565932
C6	-1.51692	0.372089	3.9633
C7	-1.54414	0.051922	2.606241
C8	-2.82825	-0.29844	1.896778
C9	-2.79549	-1.63472	1.20185
C10	-3.68521	-2.65379	1.544674
C11	-3.65389	-3.85836	0.850004
C12	-2.72906	-4.01804	-0.18013
C13	-1.8686	-2.96869	-0.47301
N14	-1.90063	-1.80455	0.204143
H15	1.624796	0.408443	1.785748
H16	1.824143	0.942572	4.22514
H17	-0.26712	0.944932	5.621213
H18	-2.44165	0.377061	4.529606
H19	-3.64703	-0.29406	2.618273
H20	-4.39987	-2.48829	2.343412
H21	-4.34358	-4.65693	1.105411
H22	-2.66942	-4.93531	-0.7549
H23	-1.13733	-3.04683	-1.26814
S24	-3.322	1.014687	0.66698
O25	-4.35262	0.385375	-0.12809
O26	-3.6542	2.175293	1.451697
O27	-2.03544	1.23448	-0.11315
O28	0.719749	1.352557	-0.2824
C29	1.717466	1.394778	-1.10534
O30	2.028998	0.614761	-1.99129
C31	2.617472	2.617349	-0.78221
F32	1.9176	3.7583	-0.70321
F33	3.211964	2.411298	0.423389
F34	3.581978	2.772237	-1.69317
H35	-0.07019	-1.06918	-2.07829
O36	1.071846	-1.49586	-0.0426
C37	1.405679	-2.08248	-1.1088
O38	0.793209	-2.0164	-2.20298
C39	2.613097	-3.03666	-1.01112
F40	3.201174	-3.19978	-2.19416
F41	3.511828	-2.58558	-0.13023
F42	2.162318	-4.2367	-0.58383

C43	-1.14778	-0.213	-2.41117
H44	-1.13447	-0.91553	-3.25754
H45	-2.17789	-0.13803	-2.07042
O46	-0.76149	1.07816	-2.88214
C47	-0.13417	1.140475	-4.06143
O48	0.069316	0.233279	-4.82652
C49	0.242163	2.607143	-4.36333
F50	0.754474	3.226422	-3.28643
F51	1.134439	2.658858	-5.35387
F52	-0.8611	3.279805	-4.745

Table S180. [Rh^{III}(DPMS)(TFA^{ax})(CH_2TFA^{eq}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	0.55585	-0.12376	-0.30791
N2	0.012268	-0.05454	1.693658
C3	0.885642	-0.38637	2.656842
C4	0.596216	-0.16223	3.997847
C5	-0.62179	0.427507	4.331105
C6	-1.52628	0.745791	3.320193
C7	-1.1896	0.483025	1.993203
C8	-2.14496	0.743939	0.8515
C9	-2.36495	-0.49943	0.025607
C10	-3.62133	-1.09356	-0.07828
C11	-3.75858	-2.29515	-0.76754
C12	-2.62779	-2.88849	-1.32161
C13	-1.4079	-2.23746	-1.20312
N14	-1.2884	-1.05984	-0.5664
H15	1.813476	-0.83338	2.322865
H16	1.319905	-0.4397	4.755899
H17	-0.87065	0.630695	5.368142
H18	-2.48597	1.19649	3.547393
H19	-3.10242	1.077687	1.254713
H20	-4.47599	-0.61383	0.38542
H21	-4.73207	-2.7673	-0.85653
H22	-2.67904	-3.83475	-1.84776
H23	-0.49702	-2.66474	-1.60011
S24	-1.59932	2.163685	-0.21203
O25	-2.40992	2.044641	-1.40291
O26	-1.73235	3.341098	0.606684
O27	-0.13727	1.832101	-0.45465
O28	2.344339	0.721562	0.330625
C29	3.019452	1.348098	-0.53606

O30	2.761923	1.419909	-1.75567
C31	4.266982	2.075939	0.008613
F32	3.894331	2.989326	0.92016
F33	5.081835	1.189336	0.605801
F34	4.940804	2.690054	-0.96427
H35	1.752572	-0.31861	-3.26841
H36	1.752185	0.599008	-1.94491
O37	1.326149	-1.98166	0.0167
C38	2.432167	-2.32904	-0.57579
O39	3.050624	-1.7504	-1.45069
C40	2.934792	-3.68312	-0.00975
F41	4.066873	-4.07265	-0.59983
F42	3.163763	-3.57875	1.317528
F43	2.008318	-4.6478	-0.19398
C44	0.86662	-0.13026	-2.65027
H45	0.320082	-1.06789	-2.6443
O46	0.099461	0.896157	-3.30383
C47	-1.14002	0.603031	-3.69508
O48	-1.704	-0.46005	-3.58423
C49	-1.77443	1.798229	-4.43958
F50	-1.32315	2.978667	-4.01241
F51	-1.46872	1.680173	-5.75316
F52	-3.1034	1.761698	-4.31906

Table S181. [Rh^{I-III}(DPMS)(H)(CH_3)(TFA^{eq})]$^{-‡}$ (no assisted deprotonation; H cis to sulfonate)

Atom	x	y	z
Rh1	0.006275	0.164808	0.00107
N2	-0.06148	0.15818	2.162353
C3	1.110729	0.247248	2.830156
C4	1.183243	0.365546	4.20903
C5	-0.00764	0.4238	4.934899
C6	-1.2097	0.340304	4.251627
C7	-1.21952	0.188896	2.853091
C8	-2.55821	0.096436	2.185646
C9	-2.74099	-0.73838	0.957529
C10	-3.97024	-1.41498	0.835647
C11	-4.22689	-2.23476	-0.24848
C12	-3.2302	-2.38535	-1.21444
C13	-2.0533	-1.67542	-1.06062
N14	-1.80543	-0.84464	-0.01809
H15	1.995153	0.272219	2.20515
H16	2.152514	0.432086	4.692671

H17	0.001906	0.540317	6.015501
H18	-2.15728	0.425207	4.769208
H19	-3.23549	-0.32193	2.932181
H20	-4.71942	-1.24741	1.599409
H21	-5.17922	-2.74983	-0.33843
H22	-3.3576	-3.03039	-2.07788
H23	-1.26198	-1.75112	-1.79227
S24	-3.40352	1.817411	1.992335
O25	-4.75517	1.413276	1.607844
O26	-3.28885	2.344241	3.350215
O27	-2.63882	2.513183	0.971507
O28	1.927703	0.945566	0.191893
C29	2.58085	1.834453	-0.4607
O30	2.287647	2.513621	-1.43586
C31	4.01789	1.986	0.122966
F32	4.81526	0.973674	-0.30755
F33	4.602851	3.13759	-0.25293
F34	4.042295	1.95117	1.478351
H42	-0.46552	1.106962	-1.11922
C36	0.275764	0.100916	-2.13053
H37	-0.6041	0.042511	-2.78026
H38	0.948263	0.878205	-2.49091
H39	0.799002	-0.86659	-2.14447

Table S182. [Rh^{I-III}(DPMS)(H)(CH_3)(TFA^{eq})]$^{-‡}$ (no assisted deprotonation; H trans to sulfonate)

Atom	x	y	z
Rh1	-0.12474	0.420083	0.008129
N2	-0.04952	0.128392	2.141738
C3	1.142716	0.195694	2.769936
C4	1.264595	0.138604	4.149849
C5	0.102318	0.038747	4.917602
C6	-1.1233	-0.0143	4.271992
C7	-1.17908	0.016887	2.86852
C8	-2.5243	-0.02321	2.205603
C9	-2.69107	-0.83906	0.958823
C10	-3.84344	-1.6348	0.851276
C11	-4.06523	-2.41594	-0.27129
C12	-3.10945	-2.39642	-1.28815
C13	-2.00295	-1.57775	-1.14031
N14	-1.7903	-0.79277	-0.05526
H15	1.999803	0.338459	2.124284
H16	2.247859	0.190439	4.60606

H17	0.152747	0.012682	6.003039
H18	-2.05043	-0.05343	4.831897
H19	-3.22359	-0.4288	2.938492
H20	-4.56531	-1.60484	1.659034
H21	-4.95899	-3.02829	-0.35179
H22	-3.21392	-2.99788	-2.18547
H23	-1.23882	-1.52966	-1.90367
S24	-3.25579	1.72603	1.990229
O25	-4.60425	1.416649	1.521663
O26	-3.17517	2.244278	3.352627
O27	-2.38617	2.376053	1.015794
O28	1.620226	1.538321	0.237783
C29	2.646901	1.517337	-0.52997
O30	2.828547	1.031941	-1.64073
C31	3.848149	2.217266	0.170498
F32	4.251815	1.48854	1.250971
F33	4.918353	2.339041	-0.63733
F34	3.543886	3.452505	0.62146
H36	0.370282	-0.0418	-1.39632
C36	-0.43698	1.176722	-1.96114
H37	-1.06876	0.601625	-2.64567
H38	-1.02123	2.012965	-1.55916
H39	0.446688	1.543012	-2.48242

Table S183. [Rh^{I-III}(DPMS)(CH_3)(H-TFA^{eq})]$^{-‡}$ (TFA^{eq} assisted deprotonation; H cis to sulfonate)

Atom	x	y	z
Rh1	-0.01244	-0.08174	0.054323
N2	-0.08896	-0.09723	2.131832
C3	1.082051	-0.14323	2.811914
C4	1.16809	-0.00036	4.186631
C5	-0.00854	0.208059	4.910588
C6	-1.21114	0.238739	4.221938
C7	-1.2367	0.066993	2.827211
C8	-2.5695	0.094416	2.143142
C9	-2.79419	-0.78567	0.949696
C10	-4.06854	-1.36854	0.830771
C11	-4.35775	-2.24612	-0.20066
C12	-3.34427	-2.54271	-1.11309
C13	-2.11962	-1.91328	-0.97015
N14	-1.83614	-1.0259	0.016329
H15	1.965928	-0.27404	2.201434
H16	2.138605	-0.04245	4.671464

H17	0.013737	0.345156	5.988372
H18	-2.14694	0.432976	4.731908
H19	-3.29545	-0.23236	2.890464
H20	-4.82415	-1.08736	1.554306
H21	-5.34421	-2.6934	-0.28764
H22	-3.49358	-3.24063	-1.93126
H23	-1.32127	-2.09693	-1.67371
S24	-3.23163	1.875558	1.895696
O25	-4.59187	1.607157	1.429723
O26	-3.14982	2.393773	3.261752
O27	-2.34745	2.509181	0.930122
O28	1.852723	1.01172	0.23223
C29	1.898925	1.994366	-0.52348
O30	1.076491	2.254282	-1.46789
C31	3.078649	2.97029	-0.39284
F32	4.044501	2.635626	-1.28105
F33	2.711523	4.236003	-0.64545
F34	3.620243	2.926931	0.834008
H42	0.450104	1.290608	-1.54936
C36	0.079831	-0.13494	-2.19198
H37	-0.92384	-0.08638	-2.62742
H38	0.764988	0.312999	-2.92721
H39	0.407183	-1.18355	-2.1469

Table S184. $[Rh^{I-III}(DPMS)(H)(CH_3)(TFAH^{eq})]^{‡}$ (no assisted deprotonation; H cis to sulfonate)

Atom	x	y	z
Rh1	0.176399	-0.32217	-0.07183
N2	0.07824	-0.08806	2.068363
C3	1.184763	-0.27218	2.815264
C4	1.178101	-0.13799	4.198124
C5	-0.01325	0.220912	4.826887
C6	-1.1492	0.426939	4.050928
C7	-1.07682	0.257658	2.664972
C8	-2.29658	0.514693	1.812568
C9	-2.66927	-0.5406	0.792272
C10	-4.0107	-0.93151	0.716337
C11	-4.40132	-1.93227	-0.16496
C12	-3.4266	-2.54086	-0.95221
C13	-2.11567	-2.09808	-0.84859
N14	-1.736	-1.10653	-0.01389
H15	2.091257	-0.5016	2.26608
H16	2.091548	-0.29816	4.760339

H17	-0.05547	0.348914	5.90424
H18	-2.08364	0.735807	4.505711
H19	-3.14366	0.575898	2.500653
H20	-4.73936	-0.43306	1.345426
H21	-5.44204	-2.23419	-0.22854
H22	-3.66901	-3.33971	-1.64455
H23	-1.32849	-2.52794	-1.45381
S24	-2.36542	2.271402	1.180995
O25	-3.69074	2.394065	0.637836
O26	-1.95454	3.065307	2.310083
O27	-1.36512	2.385393	0.008593
O28	2.023647	0.636814	-0.0154
C29	2.036961	1.878281	0.253745
O30	1.096729	2.680054	0.402314
C31	3.470611	2.425122	0.462877
F32	3.486287	3.746176	0.665201
F33	4.020714	1.829549	1.547765
F34	4.25096	2.150561	-0.59782
H35	-0.19144	0.380373	-1.38763
H43	-0.34256	2.467596	0.24093
C37	0.611397	-0.91274	-2.06232
H38	-0.1936	-1.02928	-2.7931
H39	1.411506	-0.31067	-2.49656
H40	1.010952	-1.90155	-1.79943

Table S185. $[Rh^{I-III}(DPMS)(H)(CH_3)(TFAH^{eq})]^{‡}$ (no assisted deprotonation; H trans to sulfonate)

Atom	x	y	z
Rh1	0.055887	-0.17335	-0.0703
N2	0.008976	-0.14553	2.078294
C3	1.121998	-0.38413	2.800517
C4	1.136651	-0.3169	4.186659
C5	-0.04429	0.018402	4.851549
C6	-1.19022	0.264889	4.105029
C7	-1.13783	0.169409	2.709993
C8	-2.35709	0.456148	1.872187
C9	-2.70869	-0.60511	0.854865
C10	-4.01435	-1.10799	0.83375
C11	-4.36578	-2.11728	-0.05322
C12	-3.38761	-2.61975	-0.90944
C13	-2.11466	-2.07316	-0.85934
N14	-1.775	-1.0753	-0.01225
H15	2.01048	-0.62696	2.228554

H16	2.054461	-0.52026	4.727619
H17	-0.06931	0.089663	5.934729
H18	-2.12035	0.545761	4.586311
H19	-3.20902	0.537693	2.550269
H20	-4.74619	-0.69191	1.516883
H21	-5.37829	-2.50832	-0.06994
H22	-3.59882	-3.41968	-1.61062
H23	-1.32515	-2.42708	-1.5078
S24	-2.31602	2.194789	1.18239
O25	-3.58339	2.319685	0.502061
O26	-2.06284	3.008397	2.35205
O27	-1.15927	2.194852	0.216178
O28	1.925618	0.843886	-0.00343
C29	2.053203	2.037421	0.314336
O30	1.157414	2.915936	0.566762
C31	3.49926	2.575127	0.400869
F32	3.580609	3.661385	1.175339
F33	4.313505	1.632673	0.901046
F34	3.926548	2.894578	-0.83381
H43	0.127977	2.604278	0.466345
H37	0.588209	-1.09756	-1.21523
C37	0.101581	-0.04185	-2.22241
H38	-0.40582	-0.78048	-2.8486
H39	-0.50548	0.870921	-2.20978
H40	1.085497	0.17814	-2.64085

Table S186. [Rh^{I-III}(DPMS)(H-TFA)(CH_3)(TFAH^{eq})]$^{-‡}$ (unbound TFA deprotonation; H trans to sulfonate)

Atom	x	y	z
Rh1	0.206063	-0.15085	0.00686
N2	0.100297	-0.11716	2.04504
C3	1.214019	-0.38717	2.765613
C4	1.221543	-0.36525	4.152289
C5	0.03898	-0.05561	4.828488
C6	-1.10547	0.206665	4.084708
C7	-1.05485	0.163856	2.686724
C8	-2.29128	0.440018	1.871935
C9	-2.59709	-0.56488	0.784123
C10	-3.91656	-1.0061	0.634659
C11	-4.22844	-1.98048	-0.30632
C12	-3.19387	-2.51682	-1.07216
C13	-1.9058	-2.03014	-0.90023

N14	-1.60958	-1.04684	-0.01505
H15	2.091801	-0.64009	2.180978
H16	2.1384	-0.59374	4.685942
H17	0.010146	-0.0217	5.913882
H18	-2.03948	0.467454	4.570265
H19	-3.13506	0.402282	2.565976
H20	-4.68737	-0.55958	1.252977
H21	-5.25254	-2.32217	-0.42784
H22	-3.37097	-3.304	-1.79796
H23	-1.06305	-2.42045	-1.4588
S24	-2.44511	2.2382	1.358094
O25	-3.79921	2.307581	0.840855
O26	-2.16616	2.944852	2.597456
O27	-1.43193	2.50171	0.292495
O28	1.978994	1.079136	0.085918
C29	1.93971	2.289799	0.319642
O30	0.944669	3.077301	0.523032
C31	3.280767	3.051912	0.410443
F32	3.304029	4.081545	-0.45852
F33	3.446787	3.555681	1.651281
F34	4.323273	2.257499	0.142605
H43	-0.06808	2.706104	0.465326
H37	0.832447	-1.19711	-1.64702
C37	0.364751	-0.03864	-2.24784
H38	-0.25986	-0.57168	-2.97439
H39	-0.1663	0.896396	-2.02193
H40	1.31499	0.230478	-2.72156
O44	1.193255	-2.44078	-1.76148
C45	1.939891	-2.98465	-0.8689
O46	2.686677	-2.49083	-0.03268
C47	1.804825	-4.53612	-0.91062
F48	2.581539	-5.15111	0.001777
F49	0.524398	-4.91766	-0.66512
F50	2.139453	-5.03994	-2.1232

Table S187. $Rh^{III}(DPMS)(H^{ax})(CH_3{}^{eq})(TFAH^{eq})$

Atom	x	y	z
Rh1	0.020717	-0.10882	-0.02756
N2	-0.03792	-0.18881	2.218451
C3	1.027265	-0.4781	2.983336
C4	0.977641	-0.45133	4.372812
C5	-0.22564	-0.10656	4.988281

C6	-1.32929	0.190766	4.194682
C7	-1.20377	0.137113	2.80335
C8	-2.37642	0.465517	1.904503
C9	-2.72563	-0.61418	0.903675
C10	-4.00423	-1.1789	0.922537
C11	-4.32989	-2.2042	0.042332
C12	-3.35513	-2.65668	-0.84392
C13	-2.10689	-2.05065	-0.82977
N14	-1.79739	-1.0414	0.010717
H15	1.936614	-0.73293	2.448128
H16	1.862026	-0.69246	4.952795
H17	-0.3031	-0.06827	6.07073
H18	-2.27677	0.47356	4.640506
H19	-3.25292	0.613975	2.53896
H20	-4.73466	-0.8032	1.630402
H21	-5.32209	-2.64469	0.053845
H22	-3.54972	-3.46275	-1.54276
H23	-1.31792	-2.35877	-1.50126
S24	-2.20528	2.145574	1.132916
O25	-3.44964	2.344802	0.430312
O26	-1.87218	3.021495	2.233428
O27	-1.03772	1.977516	0.174785
O28	1.923094	0.862054	0.023918
C29	2.099446	2.07654	0.176469
O30	1.224442	3.010256	0.316132
C31	3.546066	2.613444	0.215232
F32	3.755795	3.276688	1.364461
F33	4.430723	1.616189	0.130418
F34	3.746624	3.457743	-0.80827
H43	0.240474	2.656213	0.30158
H37	0.731626	-1.44772	-0.221
C37	0.037427	0.057004	-2.07798
H38	-0.3662	-0.81757	-2.59835
H39	-0.57681	0.931022	-2.32342
H40	1.065022	0.217098	-2.4194

Table S188. $Rh^{III}(DPMS)(H^{eq})(CH_3{}^{ax})(TFAH^{eq})$

Atom	x	y	z
Rh1	0.034594	-0.14123	-0.03321
N2	-0.00909	-0.20131	2.226597
C3	1.058718	-0.49382	2.983474
C4	1.011906	-0.49475	4.373778

C5	-0.19461	-0.17552	4.996176
C6	-1.30192	0.127589	4.208951
C7	-1.17635	0.103258	2.816832
C8	-2.34669	0.445986	1.922732
C9	-2.71827	-0.60814	0.902141
C10	-4.012	-1.13784	0.905576
C11	-4.37789	-2.09809	-0.03036
C12	-3.43233	-2.51262	-0.9655
C13	-2.1654	-1.94804	-0.92886
N14	-1.80918	-1.01879	-0.01785
H15	1.970805	-0.7291	2.443333
H16	1.89996	-0.73681	4.947926
H17	-0.27161	-0.16027	6.079357
H18	-2.25178	0.39087	4.661818
H19	-3.2202	0.602713	2.559271
H20	-4.72382	-0.78246	1.642362
H21	-5.38217	-2.51037	-0.03113
H22	-3.66511	-3.25467	-1.72117
H23	-1.39817	-2.22294	-1.6393
S24	-2.15446	2.127073	1.152834
O25	-3.4151	2.361413	0.491404
O26	-1.76307	2.990765	2.244248
O27	-1.02289	1.933173	0.155536
O28	1.932822	0.833381	-0.0074
C29	2.109443	2.052167	0.11135
O30	1.234083	2.987961	0.221828
C31	3.570264	2.551653	0.10098
F32	3.677448	3.789762	0.591098
F33	4.337271	1.731364	0.835708
F34	4.029053	2.546483	-1.16202
H35	0.030986	-0.11775	-1.58005
H43	0.252149	2.6254	0.226611
C37	1.021932	-1.92508	-0.20831
H38	0.758528	-2.46748	-1.12119
H39	2.093585	-1.70351	-0.23178
H40	0.789863	-2.55065	0.661741

Table S189. [Rh^{I}(DPMS)(TFAH)(CH$_3$)]$^-$

Atom	x	y	z
Rh1	0.144779	-0.30491	-0.01884
N2	0.052671	-0.18348	2.108802
C3	1.141211	-0.4309	2.870358

C4	1.129171	-0.37567	4.256718
C5	-0.0654	-0.04965	4.903224
C6	-1.18773	0.209542	4.123903
C7	-1.10409	0.138504	2.728094
C8	-2.31288	0.457607	1.887508
C9	-2.67273	-0.54727	0.817128
C10	-4.00593	-0.96455	0.731996
C11	-4.39498	-1.92105	-0.19951
C12	-3.41438	-2.44952	-1.03938
C13	-2.11256	-1.98543	-0.9302
N14	-1.72685	-1.03979	-0.03353
H15	2.04193	-0.67747	2.317608
H16	2.038202	-0.58505	4.81281
H17	-0.11794	0.00903	5.986899
H18	-2.12873	0.495171	4.581965
H19	-3.16455	0.484803	2.57218
H20	-4.73315	-0.51142	1.397178
H21	-5.43025	-2.2437	-0.26556
H22	-3.64779	-3.2082	-1.78071
H23	-1.32692	-2.34363	-1.58088
S24	-2.35552	2.257448	1.347129
O25	-3.71049	2.40559	0.84354
O26	-2.03096	2.961442	2.579462
O27	-1.34196	2.455776	0.273159
O28	2.01433	0.768205	0.011166
C29	2.039107	1.99076	0.166282
O30	1.089911	2.844191	0.330404
C31	3.416116	2.688854	0.187497
F32	3.617177	3.311326	1.368387
F33	4.419291	1.816222	0.009062
F34	3.49944	3.61938	-0.78481
C35	0.282426	-0.42189	-2.09396
H36	0.658379	-1.41131	-2.41199
H37	-0.67894	-0.2492	-2.60181
H38	0.992494	0.325382	-2.48102
H39	0.063088	2.525174	0.344635

Table S190. [Rh^{III}(DPMS)($TFAH^{eq}$)(CH_3^{eq})]$^+$

Atom	x	y	z
Rh1	-0.08024	0.051008	-0.03851
N2	-0.0776	-0.15761	2.244459
C3	0.997318	-0.42153	3.006017

C4	0.96658	-0.33221	4.3949
C5	-0.22093	0.057811	5.011287
C6	-1.33648	0.333642	4.221131
C7	-1.23066	0.210646	2.836355
C8	-2.41847	0.492874	1.933584
C9	-2.76065	-0.62699	0.97762
C10	-3.96038	-1.32806	1.082517
C11	-4.24461	-2.3531	0.183014
C12	-3.31821	-2.65521	-0.81323
C13	-2.14451	-1.91678	-0.87831
N14	-1.87286	-0.93047	0.000921
H15	1.903517	-0.70474	2.479078
H16	1.856116	-0.55799	4.972516
H17	-0.28073	0.147739	6.091392
H18	-2.27245	0.647432	4.670928
H19	-3.29366	0.692026	2.557083
H20	-4.66549	-1.06312	1.862585
H21	-5.17758	-2.9026	0.256509
H22	-3.49728	-3.44	-1.53928
H23	-1.40306	-2.09895	-1.64754
S24	-2.25177	2.073673	1.004084
O25	-3.34817	2.107518	0.081721
O26	-2.0298	3.127002	1.953514
O27	-0.88364	1.865489	0.223295
O28	1.856212	0.87498	-0.01166
C29	2.188843	2.051168	0.207693
O30	1.409412	3.056087	0.416816
C31	3.694892	2.386435	0.310964
F32	4.043931	2.280453	1.604056
F33	4.403443	1.517842	-0.40761
F34	3.931397	3.623824	-0.11215
C35	-0.13698	0.302425	-2.06824
H36	0.411712	-0.56209	-2.46936
H37	-1.16684	0.328223	-2.42658
H38	0.375901	1.228005	-2.33374
H39	0.440854	2.776835	0.399213

Table S191. $Rh^{III}(DPMS)(TFA^{eq})(CH_3^{eq})$

Atom	x	y	z
Rh1	-0.12023	0.28875	-0.01937
N2	-0.09106	-0.08243	2.252965
C3	1.031443	-0.22685	2.970529

C4	1.026001	-0.21323	4.363255
C5	-0.1861	-0.02105	5.023142
C6	-1.34665	0.159058	4.27287
C7	-1.26246	0.123697	2.880022
C8	-2.48159	0.371265	2.012896
C9	-2.7575	-0.69663	0.983528
C10	-3.87077	-1.53275	1.077801
C11	-4.10823	-2.48113	0.087002
C12	-3.22649	-2.56756	-0.98865
C13	-2.13852	-1.7053	-1.02661
N14	-1.90364	-0.79955	-0.05883
H15	1.949364	-0.31265	2.39759
H16	1.954477	-0.3353	4.910281
H17	-0.22805	0.003587	6.107997
H18	-2.30135	0.34099	4.755193
H19	-3.35927	0.471378	2.655371
H20	-4.54538	-1.42718	1.920512
H21	-4.97192	-3.13588	0.149963
H22	-3.37488	-3.28204	-1.7905
H23	-1.43006	-1.71949	-1.84713
S24	-2.40029	2.019526	1.161177
O25	-3.46421	1.975212	0.187831
O26	-2.43412	3.016618	2.200785
O27	-0.99999	2.018474	0.521683
O28	1.790553	0.886343	0.16828
C29	2.330673	2.024949	-0.17057
O30	1.845607	2.970059	-0.75578
C31	3.812469	2.057917	0.291032
F32	4.36317	3.260397	0.101166
F33	3.918144	1.753585	1.60645
F34	4.54142	1.148455	-0.39348
C35	-0.2108	0.754054	-2.00392
H36	0.401425	-0.00148	-2.51965
H37	-1.24477	0.72954	-2.357
H38	0.220267	1.746672	-2.12637

Table S192. $Rh^{III}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq})$

Atom	x	y	z
Rh1	0.023077	-0.13638	0.095069
N2	-0.57214	-0.74914	2.205068
C3	0.267939	-1.25777	3.114335
C4	-0.08741	-1.4188	4.449788

C5	-1.36349	-1.02243	4.846883
C6	-2.23746	-0.49691	3.898086
C7	-1.8106	-0.37838	2.573406
C8	-2.72003	0.178357	1.498332
C9	-2.85377	-0.7093	0.286738
C10	-4.08126	-1.28178	-0.05057
C11	-4.18377	-2.09651	-1.17267
C12	-3.04467	-2.33284	-1.93905
C13	-1.8499	-1.73763	-1.56009
N14	-1.7618	-0.93815	-0.47929
H15	1.251189	-1.53717	2.748809
H16	0.622021	-1.83817	5.154985
H17	-1.67579	-1.12232	5.882062
H18	-3.23498	-0.17409	4.175928
H19	-3.71408	0.330212	1.923232
H20	-4.94606	-1.07718	0.570423
H21	-5.13643	-2.54204	-1.44182
H22	-3.06961	-2.96693	-2.81809
H23	-0.93187	-1.90655	-2.10473
S24	-2.23036	1.890896	0.97294
O25	-3.10461	2.179076	-0.14167
O26	-2.33384	2.702129	2.161722
O27	-0.78143	1.717902	0.55592
O28	1.769264	0.776394	0.918287
C29	2.884211	1.081844	0.483195
O30	3.52418	0.583891	-0.51185
C31	3.668354	2.205401	1.199639
F32	3.898551	3.209165	0.339725
F33	2.990361	2.675751	2.245644
F34	4.850422	1.730286	1.62948
C35	0.377426	0.57535	-1.80232
H36	0.771418	-0.212	-2.45104
H37	-0.56845	0.960279	-2.18935
H38	1.095077	1.396317	-1.73658
H39	3.100664	-0.31009	-0.88146
O40	0.799932	-2.01795	-0.30253
C41	1.850504	-2.33418	-0.93856
O42	2.812759	-1.63979	-1.30602
C43	1.862314	-3.8338	-1.33136
F44	0.87432	-4.05888	-2.22956
F45	3.019494	-4.20249	-1.88414
F46	1.632855	-4.6135	-0.26058

Table S193. $[Rh^{IV}(DPMS)(TFA^{eq})(CH_3^{eq})]^+$

Atom	x	y	z
Rh1	0.029724	0.108143	-0.12308
N2	-0.02213	-0.3172	2.106867
C3	1.074597	-0.67105	2.796596
C4	1.127291	-0.57326	4.184088
C5	0.015514	-0.07844	4.862383
C6	-1.11906	0.28845	4.137921
C7	-1.10822	0.154453	2.75139
C8	-2.31311	0.517105	1.905748
C9	-2.70051	-0.58717	0.956202
C10	-3.90243	-1.28141	1.079739
C11	-4.1953	-2.31347	0.19147
C12	-3.27313	-2.6338	-0.8046
C13	-2.09828	-1.89961	-0.88472
N14	-1.82237	-0.89864	-0.02372
H15	1.92232	-1.02541	2.220224
H16	2.027968	-0.8692	4.710183
H17	0.027984	0.022625	5.943044
H18	-1.99791	0.681887	4.637237
H19	-3.15818	0.749836	2.557198
H20	-4.59941	-1.0074	1.864026
H21	-5.13008	-2.85871	0.274891
H22	-3.45762	-3.42978	-1.51703
H23	-1.36188	-2.10101	-1.65481
S24	-2.06429	2.085036	0.952958
O25	-3.01289	2.035681	-0.12364
O26	-2.03555	3.174191	1.88435
O27	-0.58692	1.909144	0.441569
O28	1.833936	0.767376	-0.25237
C29	2.217591	2.064892	-0.28884
O30	1.888989	2.831125	-1.15225
C31	3.177102	2.41206	0.870136
F32	3.443273	3.709544	0.887565
F33	2.598888	2.060307	2.04009
F34	4.315928	1.716695	0.739684
C35	-0.50435	0.589947	-2.08125
H36	-0.2141	-0.27378	-2.68536
H37	-1.56891	0.811622	-2.10055
H38	0.107768	1.473919	-2.26635

Table S194. [Rh^{II}(DPMS)(TFA^{eq})(CH_3^{eq})]$^-$

Atom	x	y	z
Rh1	-0.0876	0.310159	-0.03082
N2	-0.10062	0.122422	2.197068
C3	1.046379	0.060598	2.89282
C4	1.072712	-0.04063	4.279729
C5	-0.14026	-0.06062	4.968305
C6	-1.32498	0.031664	4.246068
C7	-1.277	0.123162	2.848963
C8	-2.54396	0.286875	2.04853
C9	-2.75933	-0.70431	0.936299
C10	-3.91372	-1.49835	0.936534
C11	-4.13965	-2.41287	-0.08381
C12	-3.19463	-2.51569	-1.10399
C13	-2.07707	-1.69439	-1.0585
N14	-1.8529	-0.80615	-0.06651
H15	1.950133	0.131193	2.294697
H16	2.023662	-0.0913	4.800833
H17	-0.16257	-0.13409	6.052668
H18	-2.28565	0.049504	4.750171
H19	-3.38792	0.198503	2.735459
H20	-4.62866	-1.37961	1.743588
H21	-5.03331	-3.0309	-0.08402
H22	-3.31587	-3.21243	-1.92726
H23	-1.32204	-1.72203	-1.83422
S24	-2.72293	2.054738	1.421565
O25	-4.03287	2.028414	0.783627
O26	-2.62742	2.835277	2.647323
O27	-1.59126	2.223748	0.493999
O28	1.9003	0.963028	0.172212
C29	2.539845	1.95921	-0.31989
O30	2.214421	2.829304	-1.11431
C31	4.005962	1.971935	0.213401
F32	4.625065	3.146956	-0.00598
F33	4.079476	1.731062	1.548494
F34	4.750029	1.011303	-0.39485
C35	-0.04463	0.500645	-2.07947
H36	0.515636	-0.33893	-2.52594
H37	-1.0541	0.526188	-2.51011
H38	0.474719	1.432633	-2.31477

Table S195. $Rh^{II}(DPMS)(TFAH^{eq})(CH_3^{eq})$

Atom	x	y	z
Rh1	0.027128	-0.1046	-0.0296
N2	-0.01673	-0.1746	2.207493
C3	1.058587	-0.44902	2.965357
C4	1.017009	-0.44434	4.354837
C5	-0.19036	-0.1353	4.981337
C6	-1.30287	0.152188	4.196862
C7	-1.18611	0.121719	2.803566
C8	-2.36971	0.452161	1.921634
C9	-2.73988	-0.61283	0.911909
C10	-4.0283	-1.15573	0.928002
C11	-4.3792	-2.14909	0.020788
C12	-3.42424	-2.58512	-0.89529
C13	-2.16639	-1.99829	-0.87511
N14	-1.82597	-1.03282	0.002976
H15	1.973929	-0.66924	2.424219
H16	1.910468	-0.67279	4.925954
H17	-0.26322	-0.11456	6.064589
H18	-2.25285	0.411103	4.651839
H19	-3.23641	0.595444	2.570736
H20	-4.74745	-0.78708	1.651081
H21	-5.37833	-2.57372	0.029816
H22	-3.64389	-3.35899	-1.62262
H23	-1.39677	-2.28395	-1.58126
S24	-2.21569	2.148618	1.169611
O25	-3.47548	2.347887	0.494168
O26	-1.8743	3.003038	2.285487
O27	-1.06457	2.017449	0.1884
O28	1.952954	0.860453	0.010655
C29	2.112548	2.071436	0.205188
O30	1.224006	2.986696	0.374814
C31	3.556987	2.617354	0.225114
F32	3.681364	3.632006	1.089284
F33	4.418246	1.652056	0.5726
F34	3.880153	3.057991	-1.00362
C35	0.053693	-0.06188	-2.08413
H36	0.504829	-0.99413	-2.45757
H37	-0.95371	0.046094	-2.49996
H38	0.665748	0.777884	-2.43109
H39	0.235995	2.633286	0.342367

Rh(DPES) complexes in TFAH

Table S196. [Rh^{I}(DPES)(TFA)(TFAH)]$^{-}$

Atom	x	y	z
Rh1	0.019813	-0.27654	-0.01642
N2	0.003906	-0.22994	2.006325
C3	1.166349	-0.54636	2.62614
C4	1.311587	-0.57323	4.00215
C5	0.203642	-0.25756	4.78497
C6	-0.98559	0.074765	4.151777
C7	-1.08945	0.090748	2.749165
C8	-2.39094	0.490203	2.065816
C9	-2.81077	-0.45563	0.944809
C10	-4.14708	-0.87998	0.829364
C11	-4.54924	-1.7394	-0.18292
C12	-3.60033	-2.17934	-1.10228
C13	-2.29891	-1.73021	-0.96218
N14	-1.90469	-0.89152	0.027094
H15	1.995903	-0.75832	1.965995
H16	2.270944	-0.83491	4.436794
H17	0.261206	-0.26302	5.870089
H18	-1.84365	0.332767	4.753165
C19	-3.52719	0.643159	3.100444
H20	-4.8814	-0.52778	1.536943
H21	-5.58728	-2.05348	-0.25118
H22	-3.85243	-2.84932	-1.91795
H23	-1.52695	-1.99986	-1.66942
S24	-2.24198	2.326153	1.391885
O25	-3.57799	2.523124	0.83287
O26	-1.96519	3.052499	2.630835
O27	-1.15813	2.347127	0.417998
O28	2.049474	0.460728	0.050533
C29	2.484542	1.565361	-0.29414
O30	2.074982	2.363525	-1.20516
C31	3.740276	2.099202	0.430612
F32	4.786407	2.159693	-0.42345
F33	3.532513	3.334627	0.913994
F34	4.095225	1.305131	1.454261
O35	-0.01823	-0.46276	-2.14541

C36	0.07953	0.436745	-3.00882
O37	0.555623	1.597259	-2.93224
C38	-0.41918	0.052501	-4.42488
F39	-1.13197	1.045103	-4.98619
F40	0.634498	-0.20264	-5.23742
F41	-1.19345	-1.05014	-4.41593
H43	1.291421	1.972063	-1.87602
H44	-4.4132	1.043068	2.60976
H45	-3.77196	-0.30692	3.591916
H46	-3.24288	1.383695	3.845896

Table S197. $Rh^{I}(DPES)(TFAH)_2$

Atom	x	y	z
Rh1	0.046481	-0.21679	0.029317
N2	-0.0261	-0.17699	2.040112
C3	1.095822	-0.48879	2.729678
C4	1.170582	-0.42214	4.111609
C5	0.038431	-0.01486	4.812166
C6	-1.11598	0.297233	4.102611
C7	-1.14784	0.207652	2.703492
C8	-2.42453	0.524904	1.909818
C9	-2.76323	-0.57198	0.888873
C10	-4.05337	-1.11337	0.799683
C11	-4.34273	-2.12234	-0.11225
C12	-3.32761	-2.5945	-0.93984
C13	-2.07006	-2.02472	-0.82264
N14	-1.7926	-1.03571	0.058501
H15	1.942329	-0.78946	2.125047
H16	2.094496	-0.68453	4.61548
H17	0.047523	0.060184	5.895242
H18	-1.99206	0.61817	4.645416
H19	-3.39971	1.561133	3.559329
H20	-4.84155	-0.74401	1.438018
H21	-5.34722	-2.53012	-0.17071
H22	-3.49666	-3.38515	-1.66285
H23	-1.23977	-2.33886	-1.44287
S24	-2.33745	2.258014	1.08604
O25	-3.61714	2.370297	0.422906
O26	-2.01692	3.132606	2.191778
O27	-1.21517	2.287218	0.058226

O28	1.967125	0.7642	0.049595
C29	2.121005	1.966221	0.278646
O30	1.229701	2.884603	0.460221
C31	3.554048	2.532788	0.382407
F32	3.750837	3.465962	-0.56188
F33	3.733108	3.099242	1.587629
F34	4.46186	1.565498	0.226609
O35	0.025837	-0.18238	-2.12796
C36	-0.62729	0.622742	-2.7959
O37	-1.33353	1.630746	-2.40059
C38	-0.657	0.472957	-4.33269
F39	-0.10899	1.553357	-4.91062
F40	0.020296	-0.61116	-4.71952
F41	-1.9267	0.359263	-4.75605
H42	-1.33146	1.811527	-1.3846
H43	0.246837	2.581954	0.37469
C44	-3.61519	0.739974	2.877463
H45	-4.50421	1.028703	2.319238
H46	-3.82347	-0.16742	3.452612

Table S198. [Rh^{III}(DPES)$(TFA)_3$]$^-$

Atom	x	y	z
Rh1	-0.08841	-0.05908	0.023172
N2	-0.14761	-0.08051	2.099517
C3	1.015248	-0.16962	2.77225
C4	1.041014	-0.29439	4.156959
C5	-0.16422	-0.33397	4.847145
C6	-1.35767	-0.23637	4.136421
C7	-1.33354	-0.10487	2.745143
C8	-2.61001	0.017378	1.913026
C9	-2.73637	-1.12878	0.90999
C10	-3.87803	-1.93303	0.842437
C11	-3.96713	-2.94152	-0.11333
C12	-2.91437	-3.12996	-0.99997
C13	-1.79981	-2.30541	-0.8961
N14	-1.71688	-1.3484	0.045977
H15	1.918979	-0.12563	2.16725
H16	1.996249	-0.36111	4.665919
H17	-0.18468	-0.43703	5.928804
H18	-2.30079	-0.25876	4.664173

O19	1.319031	-1.51898	0.275884
H20	-4.69908	-1.76588	1.525251
H21	-4.85607	-3.56455	-0.16265
H22	-2.93958	-3.89459	-1.76842
H23	-0.94034	-2.39582	-1.54982
S24	-2.56009	1.667789	0.972023
O25	-3.88744	1.806002	0.405873
O26	-2.16624	2.627647	1.983387
O27	-1.5329	1.460652	-0.10626
O28	1.297712	1.439451	-0.14153
C29	2.545026	1.442497	0.158284
O30	3.2075	0.715388	0.891407
C31	3.279559	2.661697	-0.4703
F32	4.531721	2.333089	-0.84012
F33	2.658891	3.183048	-1.53872
F34	3.384693	3.649423	0.458635
O35	-0.21808	-0.13714	-2.01081
C36	0.803593	-0.1658	-2.80609
O37	1.998939	-0.11787	-2.58713
C38	0.29712	-0.30042	-4.27196
F39	1.314141	-0.40639	-5.14345
F40	-0.47944	-1.40138	-4.4232
F41	-0.44568	0.765491	-4.64384
C43	1.585291	-2.54216	-0.45649
O44	1.058852	-2.97298	-1.47338
C45	2.793986	-3.32036	0.144132
F46	3.955955	-2.69245	-0.10314
F47	2.679517	-3.4594	1.486658
F48	2.878976	-4.56066	-0.37533
C49	-3.8554	0.144122	2.805314
H50	-4.73297	0.329854	2.186288
H51	-4.02015	-0.75549	3.407425
H52	-3.73758	1.001192	3.470486

Table S199. $Rh^{III}(DPES)(TFA)_2(TFAH^{eq})$

Atom	x	y	z
Rh1	0.130149	-0.03988	-0.09016
N2	0.068238	-0.06124	1.952127
C3	1.215644	-0.18362	2.641677
C4	1.240708	-0.11716	4.028433

C5	0.039257	0.088734	4.699688
C6	-1.14303	0.200977	3.971494
C7	-1.11986	0.114413	2.577015
C8	-2.38704	0.192481	1.723057
C9	-2.49548	-1.02542	0.803511
C10	-3.59406	-1.88772	0.815545
C11	-3.6383	-2.97606	-0.05217
C12	-2.57961	-3.1969	-0.9268
C13	-1.50896	-2.31473	-0.90409
N14	-1.48427	-1.2665	-0.0615
H15	2.109858	-0.32139	2.049168
H16	2.182678	-0.21737	4.555049
H17	0.015074	0.159073	5.782858
H18	-2.07961	0.357944	4.487702
O19	1.27105	-1.71564	-0.05887
H20	-4.41554	-1.70769	1.494318
H21	-4.49524	-3.64263	-0.04066
H22	-2.5709	-4.03139	-1.61844
H23	-0.65214	-2.42081	-1.55371
S24	-2.35604	1.749174	0.642249
O25	-3.44683	1.555158	-0.28397
O26	-2.41647	2.854408	1.568406
O27	-0.99839	1.698359	-0.03839
O28	1.825223	1.183425	0.155646
C29	2.079073	2.332126	-0.25758
O30	1.563361	2.986195	-1.21081
C31	3.156134	3.102467	0.542451
F32	3.787516	4.000765	-0.21532
F33	2.553774	3.744951	1.562115
F34	4.059832	2.256334	1.056854
O35	-0.0139	-0.19554	-2.15349
C36	-0.10524	0.741354	-2.99798
O37	0.159733	1.952318	-2.88238
C38	-0.60098	0.29928	-4.39925
F39	0.42366	0.320857	-5.26854
F40	-1.1096	-0.94404	-4.37997
F41	-1.55113	1.134284	-4.84092
H42	0.8538	2.454833	-1.87163
C43	2.325192	-1.80092	-0.83017
O44	2.825767	-0.9742	-1.56264

C45	2.927288	-3.22822	-0.71662
F46	4.038807	-3.34888	-1.44687
F47	3.230441	-3.5292	0.564066
F48	2.034845	-4.14561	-1.15429
C49	-3.65052	0.372716	2.580735
H50	-4.52162	0.473668	1.931425
H51	-3.80541	-0.47272	3.258039
H52	-3.57344	1.291651	3.16212

Table S200. $[Rh^{III}(DPES)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})]^{+}$

Atom	x	y	z
Rh1	0.198734	-0.04267	0.127924
N2	0.036199	-0.14233	2.13624
C3	1.157912	-0.30556	2.862117
C4	1.122317	-0.34396	4.247989
C5	-0.10896	-0.20612	4.881362
C6	-1.26029	-0.04114	4.113511
C7	-1.17818	-0.01269	2.720991
C8	-2.40618	0.158235	1.820778
C9	-2.50335	-0.98567	0.806847
C10	-3.64559	-1.77703	0.675264
C11	-3.67116	-2.82778	-0.23995
C12	-2.54325	-3.08909	-1.01189
C13	-1.43114	-2.27483	-0.8538
N14	-1.42982	-1.24916	0.020047
H15	2.079466	-0.40441	2.305542
H16	2.042579	-0.47764	4.805013
H17	-0.17928	-0.2266	5.964258
H18	-2.21792	0.069377	4.601947
O19	1.321013	-1.74661	0.174279
H20	-4.5157	-1.57556	1.283946
H21	-4.56378	-3.43745	-0.33904
H22	-2.51238	-3.90471	-1.72522
H23	-0.51945	-2.43719	-1.4118
S24	-2.28205	1.7982	0.916119
O25	-3.43939	1.881405	0.065708
O26	-2.02948	2.786276	1.924653
O27	-1.01956	1.613373	0.00899
O28	1.740926	1.377912	0.424745
C29	2.625319	1.83118	-0.32783

O30	3.18539	1.248304	-1.31604
C31	3.076976	3.291348	-0.07388
F32	2.192075	4.100822	-0.67633
F33	3.078837	3.5407	1.236954
F34	4.288857	3.513706	-0.57238
O35	0.366894	-0.02151	-1.998
C36	-0.21607	0.719807	-2.81097
O37	-1.0181	1.687673	-2.55045
C38	0.016243	0.435431	-4.31494
F39	-0.50904	1.387783	-5.07394
F40	1.327548	0.342174	-4.54424
F41	-0.56632	-0.73984	-4.60109
H42	2.98675	0.217655	-1.35119
C43	2.31072	-1.99283	-0.60914
O44	2.98234	-1.22266	-1.29831
C45	2.604889	-3.51429	-0.69146
F46	3.725127	-3.75958	-1.35812
F47	2.688071	-4.05051	0.532781
F48	1.571221	-4.09612	-1.34325
C49	-3.70129	0.313858	2.641704
H50	-4.54476	0.503722	1.976966
H51	-3.90587	-0.58159	3.234585
H52	-3.61683	1.171953	3.309759
H53	-1.14985	1.793391	-1.54635

Table S201. $Rh^{III}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax})$

Atom	x	y	z
Rh1	0.202462	-0.33401	0.056951
N2	0.033511	-0.09564	2.082998
C3	1.139522	-0.16902	2.84953
C4	1.107587	0.047477	4.218033
C5	-0.11538	0.354312	4.807156
C6	-1.24998	0.437597	4.008731
C7	-1.16834	0.212491	2.628577
C8	-2.384	0.342509	1.717587
C9	-2.58894	-0.89083	0.84324
C10	-3.81595	-1.56429	0.792673
C11	-3.99134	-2.65539	-0.05043
C12	-2.93334	-3.06836	-0.85409
C13	-1.73616	-2.37542	-0.77023

N14	-1.5695	-1.32941	0.063616
H15	2.060856	-0.38946	2.328577
H16	2.023116	-0.01939	4.794854
H17	-0.18908	0.534035	5.875387
H18	-2.20022	0.688366	4.456767
C19	1.266991	-2.07394	0.278623
H20	-4.63866	-1.22749	1.405941
H21	-4.94794	-3.16799	-0.08259
H22	-3.02334	-3.90289	-1.54018
H23	-0.8866	-2.62311	-1.39041
S24	-2.14997	1.878628	0.588437
O25	-3.34624	1.868014	-0.22826
O26	-1.98406	2.959521	1.539041
O27	-0.90868	1.595429	-0.18824
O28	2.029341	0.740161	0.198102
C29	2.293766	1.884603	-0.22399
O30	1.792781	2.528047	-1.19317
C31	3.389203	2.635331	0.567721
F32	2.90188	2.95975	1.781037
F33	4.454619	1.834507	0.746265
F34	3.788353	3.749691	-0.0463
O35	0.254638	-0.67624	-2.00713
C36	0.179663	0.20417	-2.91341
O37	0.452986	1.418436	-2.87664
C38	-0.28949	-0.36749	-4.2746
F39	0.691934	-1.1233	-4.80857
F40	-1.37041	-1.15501	-4.10441
F41	-0.60252	0.59467	-5.14407
H42	1.09299	1.980607	-1.84958
H43	2.29015	-1.80839	0.559115
H44	0.817156	-2.71429	1.043282
H45	1.283401	-2.58526	-0.68715
C46	-3.65545	0.691633	2.511806
H47	-4.48116	0.86084	1.820449
H48	-3.93038	-0.09685	3.220483
H49	-3.50216	1.626144	3.051494

Table S202. $[Rh^{III}(DPES)(TFAH^{eq})_2(CH_3{}^{ax})]^+$

Atom	x	y	z
Rh1	0.116581	-0.1902	0.03566

N2	0.00423	-0.14677	2.067577
C3	1.093154	-0.46346	2.800724
C4	1.098618	-0.39127	4.184925
C5	-0.06391	0.02379	4.827839
C6	-1.18064	0.352342	4.065192
C7	-1.14181	0.264849	2.669843
C8	-2.34894	0.632027	1.80341
C9	-2.70883	-0.48824	0.821117
C10	-4.00713	-0.99896	0.732041
C11	-4.31634	-1.99362	-0.19084
C12	-3.31701	-2.47206	-1.03155
C13	-2.04373	-1.93982	-0.90639
N14	-1.74971	-0.98464	-0.00042
H15	1.97038	-0.77067	2.246712
H16	1.995782	-0.65466	4.733571
H17	-0.1057	0.096009	5.910001
H18	-2.08233	0.682803	4.559687
C19	-3.56415	1.036535	2.665358
H20	-4.78425	-0.61548	1.376202
H21	-5.32832	-2.38108	-0.25224
H22	-3.50768	-3.23915	-1.77337
H23	-1.23284	-2.26319	-1.54291
S24	-1.99509	2.228122	0.84121
O25	-3.08136	2.34313	-0.09057
O26	-1.76034	3.233654	1.844175
O27	-0.6706	1.935807	0.090484
O28	2.081932	0.702318	0.027984
C29	2.336164	1.879343	0.419651
O30	1.508263	2.783139	0.719132
C31	3.836228	2.225805	0.561081
F32	4.021803	3.509917	0.826984
F33	4.345743	1.48142	1.555732
F34	4.457504	1.905098	-0.58421
H35	0.454441	2.492928	0.501237
C36	0.986226	-2.04982	0.060276
H37	0.886501	-2.5067	-0.92764
H38	2.046479	-1.91125	0.290251
H39	0.510996	-2.68156	0.813393
O40	0.092794	-0.21632	-2.09526
C41	0.981283	0.026082	-2.91473

O42	2.223844	0.317543	-2.66745
C43	0.627537	0.039368	-4.42122
F44	1.665031	-0.3661	-5.14986
F45	-0.41483	-0.76416	-4.63855
F46	0.302416	1.291937	-4.75927
H47	-4.38103	1.367997	2.023466
H48	-3.91073	0.204462	3.28452
H49	-3.30486	1.879353	3.305447
H50	2.396689	0.372624	-1.69508

Table S203. $Rh^{III}(DPES)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq})$

Atom	x	y	z
Rh1	0.015048	-0.12218	0.11026
N2	-0.6106	-0.74126	2.185506
C3	0.261979	-1.2647	3.054085
C4	-0.03657	-1.43953	4.400799
C5	-1.29246	-1.03734	4.845991
C6	-2.20042	-0.4973	3.937632
C7	-1.83758	-0.36305	2.592387
C8	-2.79714	0.196248	1.532455
C9	-2.87647	-0.72455	0.31085
C10	-4.06288	-1.37744	-0.03808
C11	-4.12222	-2.18622	-1.1679
C12	-2.98159	-2.34136	-1.9478
C13	-1.8244	-1.68578	-1.55624
N14	-1.77484	-0.90252	-0.46107
H15	1.227366	-1.54405	2.644051
H16	0.697715	-1.87036	5.072827
H17	-1.56917	-1.14246	5.89083
H18	-3.1762	-0.18212	4.280206
C19	-4.19205	0.479231	2.118994
H20	-4.94547	-1.24725	0.571465
H21	-5.0498	-2.68519	-1.43154
H22	-2.9729	-2.95867	-2.83897
H23	-0.90072	-1.79302	-2.10569
S24	-2.22633	1.893298	0.922783
O25	-3.01793	2.114909	-0.26788
O26	-2.39854	2.789172	2.042548
O27	-0.75084	1.713596	0.626558
O28	1.779455	0.755193	0.94421
C29	2.89294	1.0604	0.50523

O30	3.526197	0.566472	-0.49586
C31	3.682287	2.180319	1.221863
F32	3.886471	3.197596	0.370848
F33	3.020203	2.631398	2.286895
F34	4.876612	1.711391	1.622798
C35	0.392013	0.615151	-1.77506
H36	0.838416	-0.1487	-2.41817
H37	-0.55806	0.962259	-2.18773
H38	1.070251	1.467074	-1.6852
H39	3.096364	-0.32372	-0.86926
O40	0.779593	-2.01079	-0.3014
C41	1.828956	-2.33543	-0.93401
O42	2.799216	-1.64895	-1.29706
C43	1.82999	-3.83431	-1.32947
F44	0.839261	-4.05194	-2.22572
F45	2.984061	-4.21061	-1.88436
F46	1.597148	-4.61376	-0.2588
H47	-4.84598	0.881732	1.343677
H48	-4.64674	-0.42255	2.540312
H49	-4.11141	1.235299	2.899993

Table S204. $[Rh^{III}(DPES)\ (TFA)_2(CH_3^{ax})]^-$

Atom	x	y	z
Rh1	0.058785	-0.05031	0.081075
N2	-0.07675	-0.05916	2.141709
C3	1.052376	-0.25874	2.848806
C4	1.057273	-0.32836	4.234034
C5	-0.15276	-0.18069	4.90543
C6	-1.30662	0.06404	4.170909
C7	-1.25822	0.14097	2.771297
C8	-2.48361	0.511822	1.944178
C9	-2.8011	-0.51049	0.859725
C10	-4.08462	-1.05963	0.721601
C11	-4.3537	-1.98187	-0.28191
C12	-3.33423	-2.35042	-1.1533
C13	-2.08815	-1.76811	-0.98298
N14	-1.82727	-0.88589	-0.00175
H15	1.958316	-0.31821	2.258666
H16	1.991757	-0.48896	4.760935
H17	-0.20019	-0.23678	5.989606
H18	-2.24527	0.2106	4.685427
C19	-3.70389	0.789103	2.838355

H20	-4.87333	-0.76179	1.396911
H21	-5.35105	-2.40178	-0.38065
H22	-3.49362	-3.05573	-1.96144
H23	-1.25731	-1.99445	-1.63641
S24	-2.13812	2.22883	1.131904
O25	-3.40139	2.533983	0.482482
O26	-1.79241	3.047876	2.285194
O27	-1.01616	1.991999	0.204086
O28	1.97981	0.676937	0.30902
C29	2.444256	1.733281	-0.27644
O30	1.954289	2.493416	-1.0878
C31	3.908163	1.977525	0.197752
F32	4.38381	3.164608	-0.21455
F33	4.015815	1.952343	1.551238
F34	4.744829	1.021882	-0.2782
C36	0.927418	-1.90244	0.080397
H37	0.976476	-2.24614	-0.95623
H38	1.943809	-1.79757	0.46852
H39	0.353831	-2.60774	0.693329
O40	0.36152	-0.05894	-1.96492
C41	-0.49525	0.344632	-2.83462
O42	-1.70578	0.508557	-2.75357
C43	0.1417	0.578179	-4.23452
F44	1.479691	0.456585	-4.26936
F45	-0.36005	-0.32983	-5.11786
F46	-0.17082	1.800473	-4.70675
H47	-4.52436	1.159134	2.223678
H48	-4.03189	-0.10179	3.387286
H49	-3.45796	1.580812	3.54673

Table S205. $[Rh^{III}(DPES)\ (TFA)_2(CH_3{}^{eq})]^-$

Atom	x	y	z
Rh1	-0.04458	-0.04134	-0.17265
N2	-0.60825	-0.66754	1.939507
C3	0.318549	-1.19366	2.746281
C4	0.089907	-1.3791	4.107028
C5	-1.14305	-0.9893	4.623086
C6	-2.10517	-0.4483	3.772323
C7	-1.81136	-0.30081	2.410542
C8	-2.81793	0.272926	1.401571
C9	-2.9607	-0.63079	0.170685
C10	-4.15699	-1.3001	-0.11426

C11	-4.26507	-2.10493	-1.24385
C12	-3.16695	-2.23627	-2.08703
C13	-2.00192	-1.55863	-1.75634
N14	-1.90328	-0.78182	-0.66213
H15	1.25634	-1.45725	2.268423
H16	0.862472	-1.80664	4.737713
H17	-1.36066	-1.10341	5.681912
H18	-3.06311	-0.14092	4.169993
C19	-4.18427	0.543607	2.056143
H20	-5.00692	-1.1898	0.544423
H21	-5.19732	-2.62043	-1.45777
H22	-3.19805	-2.85133	-2.98
H23	-1.10406	-1.63025	-2.35568
S24	-2.26144	1.990868	0.809444
O25	-3.15919	2.264232	-0.29895
O26	-2.38552	2.83799	1.9809
O27	-0.82802	1.8336	0.403767
O28	1.816961	0.42483	0.573897
C29	2.52183	1.486182	0.388076
O30	2.373294	2.449001	-0.34572
C31	3.762381	1.450747	1.330945
F32	4.486051	0.316734	1.183216
F33	4.594372	2.486161	1.113138
F34	3.385037	1.510189	2.63445
C35	0.326708	0.669337	-2.06389
H36	1.05151	0.012692	-2.54655
H37	-0.61684	0.715036	-2.62082
H38	0.738519	1.668616	-1.92469
H39	-4.06749	1.290957	2.840984
O40	0.670451	-1.95035	-0.45732
C41	1.778811	-2.31023	-1.01171
O42	2.498712	-1.76733	-1.83207
C43	2.182337	-3.71792	-0.47941
F44	1.207343	-4.63636	-0.69332
F45	3.299793	-4.18303	-1.06385
F46	2.410761	-3.68717	0.857239
H47	-4.87292	0.953236	1.315094
H48	-4.6178	-0.36473	2.488111

Table S206. [Rh^{III}(DPES) (TFAH)$_2$(CH_3^{eq})]$^+$

Atom	x	y	z
Rh1	-0.15452	-0.29034	-0.03553

N2	-0.75322	-0.61436	2.13653
C3	0.074146	-1.16359	3.038371
C4	-0.21096	-1.20232	4.398165
C5	-1.40577	-0.63363	4.829256
C6	-2.26773	-0.0652	3.892825
C7	-1.92203	-0.07184	2.537735
C8	-2.84522	0.515931	1.456304
C9	-3.08759	-0.48127	0.313608
C10	-4.361	-0.99123	0.049596
C11	-4.56703	-1.88023	-1.00181
C12	-3.48659	-2.25446	-1.79316
C13	-2.23925	-1.73059	-1.49135
N14	-2.04765	-0.87592	-0.46587
H15	0.998358	-1.58105	2.64995
H16	0.486667	-1.65988	5.090902
H17	-1.67041	-0.63006	5.882063
H18	-3.19488	0.379616	4.225944
C19	-4.17528	1.023521	2.054375
H20	-5.1995	-0.69001	0.660658
H21	-5.56165	-2.2679	-1.19817
H22	-3.59434	-2.93673	-2.62864
H23	-1.36149	-1.99522	-2.06386
S24	-2.11287	2.080369	0.727795
O25	-2.9068	2.375753	-0.4316
O26	-1.97704	3.028919	1.799902
O27	-0.66459	1.655956	0.294568
O28	1.877654	0.238852	0.481771
C29	2.292761	1.348443	0.888621
O30	1.595035	2.4006	1.066149
C31	3.785081	1.475394	1.274062
F32	3.890562	1.276103	2.594673
F33	4.488904	0.533337	0.632987
F34	4.252846	2.676134	0.961191
C35	0.249119	0.20623	-1.99612
H36	0.5877	-0.67646	-2.54642
H37	-0.66265	0.613804	-2.43546
H38	1.028129	0.972239	-1.99906
H39	0.598979	2.246148	0.816687
O40	0.454946	-2.2792	-0.38561
C41	1.587343	-2.7726	-0.43062
O42	2.720386	-2.18319	-0.20791
C43	1.720306	-4.2842	-0.73121

F44	0.689686	-4.68262	-1.47841
F45	2.860215	-4.54035	-1.36513
F46	1.698846	-4.94008	0.437897
H47	-4.80727	1.442181	1.269876
H48	-4.71628	0.217967	2.557148
H49	-3.97914	1.817584	2.77528
H50	2.605821	-1.22606	0.037276

Table S207. Rh^{IV}(DPES) $(TFA)_2(CH_3^{ax})$

Atom	x	y	z
Rh1	0.100162	-0.13934	0.017694
N2	-0.0032	-0.16958	2.111638
C3	1.134213	-0.33384	2.814353
C4	1.142044	-0.36941	4.200237
C5	-0.06828	-0.22275	4.870935
C6	-1.23017	-0.00981	4.136857
C7	-1.18735	0.032803	2.738858
C8	-2.41487	0.390664	1.906598
C9	-2.74782	-0.65704	0.847109
C10	-4.01771	-1.24034	0.758976
C11	-4.29974	-2.16865	-0.23733
C12	-3.30741	-2.50594	-1.1522
C13	-2.06675	-1.9009	-1.02382
N14	-1.79792	-1.01345	-0.04757
H15	2.042164	-0.40296	2.230231
H16	2.079194	-0.50234	4.728677
H17	-0.11023	-0.25276	5.955509
H18	-2.16757	0.140899	4.652272
F19	2.012642	1.054957	-4.56025
H20	-4.78943	-0.96405	1.462276
H21	-5.28727	-2.6158	-0.2981
H22	-3.48041	-3.21588	-1.95305
H23	-1.26039	-2.09965	-1.71661
S24	-2.05609	2.063866	1.053769
O25	-3.20749	2.285807	0.208362
O26	-1.82462	2.961517	2.162586
O27	-0.8008	1.815904	0.25785
O28	1.95632	0.671014	0.274661
C29	2.427719	1.616486	-0.48634
O30	2.036836	2.008725	-1.56807
C31	3.659617	2.271138	0.194876
F32	4.26679	3.138663	-0.61786

F33	3.27643	2.930378	1.309071
F34	4.561481	1.336082	0.565359
C36	1.024051	-1.99272	0.175333
H37	0.979816	-2.43395	-0.81892
H38	2.058753	-1.79652	0.448534
H39	0.489958	-2.58992	0.915019
O40	0.079973	-0.21545	-1.93443
C41	1.138661	-0.19815	-2.74368
O42	2.127562	-0.88239	-2.63039
C43	0.867446	0.651894	-4.00898
F44	0.221977	-0.13839	-4.90472
F45	0.094676	1.711428	-3.7651
C46	-3.63429	0.707983	2.79092
H47	-4.45505	1.062283	2.165919
H48	-3.96765	-0.16612	3.359477
H49	-3.38741	1.514476	3.480969

Table S208. Rh^{IV}(DPES) $(TFA)_2(CH_3^{eq})$

Atom	x	y	z
Rh1	-0.21373	-0.25246	-0.08998
N2	-0.8042	-0.64599	2.063359
C3	0.11167	-1.13119	2.912018
C4	-0.15743	-1.27205	4.270161
C5	-1.40679	-0.87732	4.738024
C6	-2.34212	-0.35273	3.846458
C7	-2.0145	-0.24113	2.492218
C8	-2.97183	0.361942	1.455577
C9	-3.20059	-0.58008	0.269411
C10	-4.4522	-1.14478	0.005272
C11	-4.63727	-1.95539	-1.11078
C12	-3.56352	-2.19325	-1.96239
C13	-2.3387	-1.62353	-1.64712
N14	-2.1661	-0.84865	-0.56009
H15	1.073294	-1.38322	2.480766
H16	0.601556	-1.6699	4.934573
H17	-1.655	-0.96305	5.791815
H18	-3.30676	-0.02588	4.210031
F19	2.101372	-3.14774	1.183672
H20	-5.28528	-0.94478	0.664212
H21	-5.61233	-2.38905	-1.31138
H22	-3.65893	-2.80945	-2.8493
H23	-1.45873	-1.79147	-2.25386

S24	-2.23426	1.96085	0.769626
O25	-2.96108	2.202312	-0.4553
O26	-2.3133	2.923731	1.8387
O27	-0.76535	1.614978	0.520077
O28	1.695725	0.012697	0.561768
C29	2.420505	1.093969	0.469577
O30	2.235966	2.113889	-0.15967
C31	3.703349	0.920523	1.331
F32	3.388495	0.548265	2.59376
F33	4.49722	-0.03773	0.810717
F34	4.40456	2.055351	1.397905
C35	0.060562	0.709889	-1.9195
H36	0.607248	-0.0322	-2.50403
H37	-0.93303	0.945276	-2.29756
H38	0.65556	1.584554	-1.67314
O40	0.359701	-2.0439	-0.64845
C41	1.603401	-2.34333	-1.01127
O42	2.201762	-1.89898	-1.95991
C43	2.196538	-3.46557	-0.12556
F44	1.50994	-4.61027	-0.31913
F45	3.478391	-3.68352	-0.41483
C46	-4.30182	0.808365	2.087758
H47	-4.94439	1.254733	1.326382
H48	-4.83088	-0.02958	2.551091
H49	-4.1115	1.569552	2.84431

Table S209. $[Rh^{IV}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3^{ax})]^+$

Atom	x	y	z
Rh1	0.09883	-0.12778	-0.02668
N2	0.038711	-0.1387	2.052451
C3	1.164212	-0.3851	2.752777
C4	1.178208	-0.40232	4.139866
C5	-0.01092	-0.151	4.816575
C6	-1.16157	0.134587	4.084985
C7	-1.1233	0.149059	2.689679
C8	-2.34375	0.537794	1.847665
C9	-2.70856	-0.54756	0.828984
C10	-3.99108	-1.0951	0.760584
C11	-4.29418	-2.06873	-0.18967
C12	-3.30772	-2.48011	-1.0792
C13	-2.04881	-1.90516	-0.9798
N14	-1.76105	-0.97958	-0.04133

H15	2.061924	-0.55578	2.175074
H16	2.10469	-0.60715	4.664412
H17	-0.04615	-0.16053	5.901539
H18	-2.08122	0.35951	4.605861
F19	-0.44982	1.320908	-5.13076
H20	-4.76122	-0.75944	1.439659
H21	-5.29425	-2.48846	-0.23536
H22	-3.49774	-3.22314	-1.84544
H23	-1.25365	-2.15404	-1.66868
S24	-1.94047	2.148508	0.961109
O25	-3.08835	2.473592	0.149666
O26	-1.50806	3.051955	1.997107
O27	-0.76695	1.820798	0.036586
O28	2.026942	0.724784	0.141769
C29	2.425497	1.882863	-0.12049
O30	1.968698	2.710643	-0.96533
C31	3.624631	2.373695	0.725412
F32	4.60945	1.464676	0.667322
F33	4.075858	3.551818	0.313631
F34	3.208098	2.475164	2.005174
H35	1.226756	2.3284	-1.62542
C36	1.052619	-1.95361	0.038768
H37	0.968588	-2.33911	-0.97926
H38	2.098914	-1.76311	0.277353
H39	0.56927	-2.60407	0.767676
O40	0.049081	-0.27732	-2.06444
C41	0.102689	0.695969	-2.90023
O42	0.459456	1.861873	-2.70921
C43	-0.36186	0.274941	-4.31901
F44	0.511763	-0.61024	-4.82437
F45	-1.56727	-0.31994	-4.23378
C46	-3.55024	0.924821	2.728226
H47	-4.37197	1.28047	2.10496
H48	-3.8966	0.074588	3.3216
H49	-3.27757	1.738911	3.400768

Table S210. [Rh^{IV}(DPES)(TFA^{ax})($TFAH^{eq}$)(CH_3^{eq})]$^+$

Atom	x	y	z
Rh1	0.027379	-0.12761	0.062968
N2	-0.5731	-0.76542	2.149083
C3	0.307135	-1.32435	2.989941
C4	-0.00077	-1.5813	4.321566

C5	-1.26634	-1.22915	4.780222
C6	-2.17884	-0.64713	3.899522
C7	-1.80697	-0.42712	2.572151
C8	-2.76505	0.188183	1.534405
C9	-2.88051	-0.70114	0.289039
C10	-4.08688	-1.30605	-0.06723
C11	-4.16351	-2.12979	-1.18769
C12	-3.01977	-2.34812	-1.94774
C13	-1.84235	-1.72741	-1.55908
N14	-1.78196	-0.92312	-0.47809
H15	1.279794	-1.56727	2.575245
H16	0.735841	-2.03834	4.973043
H17	-1.54793	-1.40263	5.81405
H18	-3.16045	-0.36893	4.256743
F19	1.613509	-4.55648	-0.00521
H20	-4.9721	-1.13455	0.528092
H21	-5.10703	-2.5941	-1.45648
H22	-3.02437	-2.98528	-2.82483
H23	-0.92	-1.88372	-2.09954
S24	-2.16361	1.876096	1.011756
O25	-3.00861	2.313472	-0.06504
O26	-2.00458	2.65483	2.20623
O27	-0.72003	1.632323	0.420087
O28	1.784652	0.751577	0.87434
C29	2.911889	1.092356	0.475861
O30	3.586545	0.599692	-0.49401
C31	3.590035	2.279729	1.205321
F32	3.128276	3.412178	0.657009
F33	3.267669	2.253219	2.500134
F34	4.912297	2.229659	1.073627
C35	0.466508	0.496361	-1.87626
H36	0.961874	-0.31008	-2.41623
H37	-0.4832	0.77168	-2.33505
H38	1.11544	1.366918	-1.78225
H39	3.174732	-0.27221	-0.86157
O40	0.758435	-1.98236	-0.25332
C41	1.844307	-2.34891	-0.84811
O42	2.792965	-1.66537	-1.22858
C43	1.842147	-3.87376	-1.13524
F44	0.841868	-4.13377	-2.00422
F45	2.991245	-4.26947	-1.66635
C46	-4.14671	0.504019	2.145121

H47	-4.80052	0.956818	1.398394
H48	-4.61896	-0.40239	2.530426
H49	-4.03724	1.214046	2.965609

Table S211. Rh^{II}(DPES)(TFA)(TFAH)

Atom	x	y	z
Rh1	-0.00224	-0.22253	-0.01528
N2	0.010297	-0.2993	2.038922
C3	1.143573	-0.66749	2.669431
C4	1.239248	-0.71193	4.051445
C5	0.121228	-0.35109	4.798935
C6	-1.03952	0.039376	4.140984
C7	-1.08919	0.063655	2.741071
C8	-2.33223	0.514539	1.979069
C9	-2.78704	-0.52595	0.957688
C10	-4.10195	-1.00794	0.924602
C11	-4.48978	-1.93942	-0.03202
C12	-3.55829	-2.38464	-0.96565
C13	-2.27106	-1.87439	-0.901
N14	-1.90046	-0.9814	0.03894
H15	1.98584	-0.89943	2.029596
H16	2.169777	-1.01408	4.518562
H17	0.150717	-0.36572	5.884199
H18	-1.90504	0.33439	4.71607
C19	-3.47254	0.900511	2.93846
H20	-4.82525	-0.64817	1.641594
H21	-5.51191	-2.30534	-0.04901
H22	-3.81532	-3.10131	-1.73744
H23	-1.51093	-2.13822	-1.62531
S24	-1.95161	2.174151	1.086018
O25	-3.20836	2.487384	0.43685
O26	-1.51439	3.028659	2.172078
O27	-0.85844	1.865822	0.115722
O28	2.000469	0.498509	0.096013
C29	2.417198	1.633755	-0.20177
O30	1.960302	2.464572	-1.04731
C31	3.688701	2.135098	0.522236
F32	4.70536	2.22673	-0.35099
F33	3.472332	3.341919	1.058551
F34	4.046672	1.290799	1.501348

O35	-0.09276	-0.37907	-2.09925
C36	-0.04703	0.585753	-2.91712
O37	0.392501	1.740568	-2.76035
C38	-0.57853	0.256658	-4.3351
F39	-1.27399	1.283467	-4.83739
F40	0.459469	0.002835	-5.15642
F41	-1.37566	-0.82755	-4.32813
H43	1.166249	2.104207	-1.70641
H44	-4.3114	1.297812	2.366955
H45	-3.81193	0.049836	3.539005
H46	-3.13654	1.699073	3.600133

Table S212. $[Rh^{II}(DPES)(TFAH)_2]^+$

Atom	x	y	z
Rh1	-0.03253	-0.04471	0.029205
N2	-0.05346	-0.11538	2.068583
C3	1.079478	-0.43309	2.729215
C4	1.144727	-0.44011	4.114655
C5	0.000225	-0.09672	4.828762
C6	-1.16459	0.229079	4.137581
C7	-1.18613	0.211234	2.739922
C8	-2.45416	0.538578	1.937759
C9	-2.79177	-0.58351	0.944884
C10	-4.04564	-1.20085	0.917039
C11	-4.30449	-2.23042	0.015113
C12	-3.30281	-2.63946	-0.86066
C13	-2.07821	-1.99064	-0.80441
N14	-1.8371	-0.99427	0.073255
H15	1.941444	-0.6685	2.115674
H16	2.072619	-0.70301	4.609696
H17	0.007851	-0.08035	5.914034
H18	-2.05149	0.499847	4.691916
C19	-3.64759	0.835017	2.87351
H20	-4.8249	-0.88049	1.593222
H21	-5.28091	-2.70422	0.000738
H22	-3.45801	-3.43727	-1.57804
H23	-1.26487	-2.24589	-1.47395
S24	-2.26219	2.191854	1.032582
O25	-3.46876	2.342514	0.264484
O26	-1.89482	3.13932	2.050227

O27	-1.05747	2.006726	0.054138
O28	1.891646	0.877147	0.053213
C29	2.143421	2.071793	0.272814
O30	1.305461	3.039733	0.429331
C31	3.629324	2.472601	0.428399
F32	3.780662	3.791248	0.446737
F33	4.065974	1.957025	1.590957
F34	4.336509	1.949508	-0.57434
O35	-0.03991	-0.06835	-2.10402
C36	-0.6443	0.712362	-2.85521
O37	-1.31977	1.76063	-2.52645
C38	-0.63459	0.396753	-4.36962
F39	-1.19193	1.372685	-5.07598
F40	0.624179	0.209251	-4.77158
F41	-1.32898	-0.73924	-4.55235
H42	-1.32833	1.925597	-1.52676
H43	0.340428	2.740475	0.354297
H44	-4.52059	1.123624	2.287893
H45	-3.89709	-0.03754	3.483125
H46	-3.4115	1.673608	3.528752

Table S213. [Rh^{III}(DPES)(TFA^{eq})(CH_3^{ax}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	-0.02043	0.013759	0.004128
N2	-0.03555	0.019727	2.077999
C3	1.131817	0.013474	2.74649
C4	1.189293	-0.04661	4.13072
C5	-0.00929	-0.10149	4.836394
C6	-1.21187	-0.06761	4.137788
C7	-1.21297	0.007393	2.741062
C8	-2.49792	0.134407	1.925417
C9	-2.66651	-1.00121	0.918674
C10	-3.82448	-1.78384	0.869839
C11	-3.96363	-2.7732	-0.09915
C12	-2.9454	-2.96387	-1.02711
C13	-1.81573	-2.1624	-0.93965
N14	-1.67883	-1.22865	0.019051
H15	2.02703	0.063039	2.140722
H16	2.150775	-0.05043	4.631507
H17	-0.0126	-0.15852	5.920645
H18	-2.14698	-0.08612	4.679432

H20	-4.62179	-1.61303	1.579029
H21	-4.86621	-3.37582	-0.13281
H22	-3.01835	-3.70478	-1.81511
H23	-1.01106	-2.21667	-1.66096
S24	-2.40761	1.795127	0.992955
O25	-3.72874	1.987918	0.443385
O26	-1.93139	2.720096	1.995315
O27	-1.40713	1.543663	-0.11909
O28	1.461205	1.461717	0.05567
C29	2.518137	1.159392	-0.5679
O30	2.848868	0.002895	-0.9256
C31	3.532569	2.300824	-0.78055
F32	4.292999	2.077839	-1.85403
F33	2.932795	3.482708	-0.90227
F34	4.338747	2.341647	0.309049
O35	-0.14747	-0.17643	-2.02488
C36	0.322796	0.63499	-2.92548
O37	1.097609	1.566452	-2.82496
C38	-0.26704	0.252759	-4.31203
F39	0.323527	0.927919	-5.3022
F40	-0.10717	-1.07024	-4.55458
F41	-1.58951	0.513573	-4.35257
H42	1.859188	-0.78108	-0.44344
C43	1.316661	-1.89872	0.031944
H44	2.254526	-2.07606	0.571177
H45	0.530388	-2.30152	0.667353
H46	1.320536	-2.44889	-0.91216
C46	-3.7303	0.294796	2.830684
H47	-4.61181	0.493088	2.221198
H48	-3.90685	-0.59484	3.443654
H49	-3.59119	1.155965	3.486352

Table S214. $[Rh^{III}(DPES)(TFA^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	-0.12962	-0.08142	-0.05309
N2	-0.14711	-0.04657	2.049649
C3	1.017932	-0.15627	2.705625
C4	1.094722	-0.014	4.085315
C5	-0.0748	0.26543	4.784769
C6	-1.27678	0.384639	4.090342
C7	-1.29942	0.219835	2.702448
C8	-2.58642	0.32568	1.880084

C9	-2.79379	-0.92927	1.029918
C10	-3.90479	-1.76359	1.189766
C11	-4.05773	-2.89042	0.388451
C12	-3.09083	-3.17638	-0.5703
C13	-2.00776	-2.31744	-0.68379
N14	-1.86652	-1.22677	0.090996
H15	1.889733	-0.33347	2.089169
H16	2.052269	-0.10856	4.584869
H17	-0.05766	0.395009	5.862706
H18	-2.18718	0.61099	4.627541
H19	-4.65263	-1.53102	1.934603
H20	-4.92283	-3.53428	0.514728
H21	-3.16348	-4.04216	-1.21881
H22	-1.22376	-2.49269	-1.40818
S23	-2.49838	1.803513	0.69677
O24	-3.53512	1.530734	-0.27353
O25	-2.61504	2.978023	1.526321
O26	-1.09908	1.727085	0.107406
O27	1.655606	0.894427	0.079575
C28	2.007003	1.901393	-0.67064
O29	1.495233	2.342976	-1.67815
C30	3.298229	2.547113	-0.09733
F31	3.092484	2.996508	1.159683
F32	4.303053	1.642934	-0.04566
F33	3.706668	3.576836	-0.84479
H34	0.309415	0.484703	-3.03262
H35	0.776653	-0.55783	-1.95658
O36	1.00838	-1.8312	0.020715
C37	1.762985	-2.01442	-0.97234
O38	1.74341	-1.36207	-2.04639
C39	2.745997	-3.19912	-0.87962
F40	3.829333	-2.98738	-1.62864
F41	3.127146	-3.40781	0.386435
F42	2.122088	-4.30818	-1.32565
C43	-0.40318	0.128729	-2.2783
H44	-1.04222	-0.65155	-2.70001
H45	-0.98796	1.01901	-2.05603
C46	-3.8107	0.628184	2.759637
H47	-4.69903	0.728518	2.133281
H48	-3.98419	-0.15951	3.499253
H49	-3.66774	1.578031	3.274627

Table S215. $[Rh^{III}(DPES)(TFA^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Atom	x	y	z
Rh1	-0.04065	-0.14282	-0.17425
N2	-0.04219	-0.1313	1.907423
C3	1.105876	-0.34785	2.566574
C4	1.199775	-0.17481	3.941572
C5	0.066166	0.243872	4.631007
C6	-1.12373	0.448981	3.935448
C7	-1.16955	0.245297	2.553499
C8	-2.46092	0.390069	1.739241
C9	-2.70743	-0.88649	0.931459
C10	-3.84438	-1.67834	1.116499
C11	-4.00501	-2.85534	0.39182
C12	-3.01284	-3.24108	-0.50332
C13	-1.90567	-2.41844	-0.65251
N14	-1.77285	-1.26655	0.029509
H15	1.947419	-0.65616	1.959781
H16	2.142236	-0.35707	4.445411
H17	0.099572	0.405649	5.704181
H18	-2.00937	0.766668	4.467743
H20	-4.60306	-1.37737	1.824831
H21	-4.89069	-3.46637	0.537408
H22	-3.08031	-4.15964	-1.07517
H23	-1.08508	-2.68049	-1.30484
S24	-2.34897	1.836646	0.522049
O25	-3.38834	1.555581	-0.44396
O26	-2.453	3.033121	1.321949
O27	-0.95404	1.713764	-0.05523
O28	1.744301	0.908983	-0.02634
C29	2.108598	1.550752	-1.05063
O30	1.527712	1.566219	-2.15683
C31	3.381414	2.403252	-0.87024
F32	3.135998	3.389235	0.011056
F33	4.379929	1.645526	-0.38819
F34	3.775638	2.949533	-2.02222
H35	-0.15256	0.34566	-3.34201
H36	0.565662	0.685043	-2.08208
O37	0.948673	-1.92517	-0.15374
C38	1.968629	-2.13969	-0.93525
O39	2.471871	-1.42082	-1.77691
C40	2.53014	-3.56368	-0.67816
F41	3.580418	-3.82809	-1.45978

F42	2.916847	-3.70306	0.607982
F43	1.579284	-4.49423	-0.92486
C44	-0.43109	-0.19331	-2.42405
H45	-0.19147	-1.23544	-2.6248
H46	-1.49827	-0.00923	-2.30822
C46	-3.66435	0.745793	2.627623
H47	-4.55644	0.860886	2.009149
H48	-3.85237	-0.0221	3.384141
H49	-3.48857	1.701804	3.12042

Table S216. $[Rh^{III\text{-}I}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{-\ddagger}$

Atom	x	y	z
Rh1	0.184113	-0.27329	-0.13004
N2	0.095913	-0.15517	1.902844
C3	1.233754	-0.32964	2.612125
C4	1.285049	-0.19948	3.990693
C5	0.112677	0.129986	4.664001
C6	-1.0573	0.298347	3.934476
C7	-1.0661	0.146136	2.538817
C8	-2.3486	0.318792	1.730625
C9	-2.58832	-0.82901	0.751906
C10	-3.83587	-1.47139	0.677961
C11	-4.06001	-2.50464	-0.22178
C12	-3.02613	-2.89725	-1.06752
C13	-1.81466	-2.23429	-0.96702
N14	-1.59441	-1.23702	-0.08212
H15	2.117715	-0.5991	2.050192
H16	2.224813	-0.36334	4.506405
H17	0.101666	0.249097	5.743991
H18	-1.97008	0.551798	4.452216
H20	-4.63947	-1.15544	1.325616
H21	-5.03145	-2.98957	-0.26229
H22	-3.14563	-3.69285	-1.79526
H23	-0.98567	-2.46392	-1.62212
S24	-2.31717	2.025921	0.783587
O25	-3.61595	2.008826	0.119823
O26	-2.17499	2.962826	1.893053
O27	-1.1698	1.989407	-0.12587
O28	2.012232	0.884613	-0.01397
C29	2.189086	2.050654	-0.39258
O30	1.631525	2.695885	-1.34204
C31	3.276314	2.849812	0.360727

F32	4.493214	2.348381	0.058995
F33	3.273877	4.150489	0.042922
F34	3.101931	2.739744	1.688224
O35	0.185879	-0.56381	-2.24023
C36	0.067831	0.337217	-3.11043
O37	0.306949	1.561618	-3.04647
C38	-0.42851	-0.196	-4.47783
F39	-0.69477	0.784589	-5.35174
F40	0.506847	-1.00047	-5.03325
F41	-1.55175	-0.92994	-4.32599
H42	0.959088	2.126403	-1.97741
C43	1.745114	-2.30522	-0.0812
H44	2.469603	-1.51297	0.001527
H45	1.207395	-2.62467	0.795683
H46	1.385485	-2.58337	-1.05945
O47	2.986871	-3.66724	-0.02568
C48	3.767652	-3.55414	0.990637
O49	3.775816	-2.72187	1.891357
C50	4.841556	-4.68047	0.996284
F51	4.270071	-5.90647	0.988449
F52	5.637445	-4.60034	-0.09381
F53	5.634562	-4.61385	2.080452
C53	-3.56451	0.504238	2.662112
H54	-4.45036	0.7168	2.064608
H55	-3.74483	-0.3771	3.289577
H56	-3.4078	1.377933	3.293022

Table S217. $[Rh^{III\text{-}I}(DPES)(TFAH^{eq})_2(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Atom	x	y	z
Rh1	-0.02001	-0.24831	-0.2202
N2	0.087242	-0.0869	1.811262
C3	1.301472	-0.21253	2.394518
C4	1.48377	-0.10586	3.765887
C5	0.374787	0.146989	4.562232
C6	-0.87427	0.268251	3.959503
C7	-1.01395	0.142952	2.572999
C8	-2.39143	0.257566	1.899784
C9	-2.68816	-0.89834	0.925012
C10	-3.91501	-1.57333	0.963197
C11	-4.1785	-2.62561	0.092694
C12	-3.20338	-3.00128	-0.82401
C13	-2.00875	-2.29926	-0.83041

N14	-1.7544	-1.27789	0.014777
H15	2.141457	-0.44857	1.753838
H16	2.478808	-0.23679	4.175333
H17	0.467745	0.241754	5.639719
H18	-1.73677	0.459711	4.579283
H20	-4.67554	-1.28041	1.670353
H21	-5.13409	-3.1387	0.135148
H22	-3.35332	-3.81542	-1.52423
H23	-1.22279	-2.53272	-1.53552
S24	-2.5878	1.942494	1.048909
O25	-3.86497	1.881807	0.395295
O26	-2.3091	2.913733	2.074285
O27	-1.50219	2.039197	-0.07468
O28	1.732713	0.959135	-0.51102
C29	1.780754	2.164649	-0.05719
O30	0.861017	2.835671	0.418958
C31	3.199842	2.779241	-0.1081
F32	3.181555	4.089245	0.141006
F33	3.980042	2.177157	0.807381
F34	3.74385	2.580091	-1.32501
O35	-0.19893	-0.45945	-2.35042
C36	0.58101	-0.07311	-3.22287
O37	1.716297	0.532821	-3.05913
C38	0.199477	-0.26606	-4.70558
F39	1.273218	-0.56812	-5.44121
F40	-0.70156	-1.24612	-4.82547
F41	-0.33746	0.874944	-5.16678
H42	-0.58823	2.405485	0.232532
C43	1.434946	-2.11842	-0.15685
H44	2.246938	-1.41179	-0.17374
H45	1.03027	-2.46102	0.779913
H46	1.107811	-2.58806	-1.07328
O47	2.822773	-3.54918	0.019608
C48	3.641019	-3.20703	0.941656
O49	3.648571	-2.1994	1.653923
C50	4.750078	-4.27628	1.164856
F51	5.740525	-3.81354	1.944007
F52	4.228451	-5.36773	1.770919
F53	5.295984	-4.67847	0.000179
H54	1.891556	0.712993	-2.07925
C54	-3.51049	0.360377	2.967758
H55	-4.47402	0.531368	2.48974

H56	-3.55959	-0.5524	3.567778
H57	-3.33178	1.213441	3.619976

Table S218. [Rh^{III-II}(DPES)(TFA^{eq})($TFAH^{eq}$)(CH_3^{ax}-$OVCl_3$)]‡

Atom	x	y	z
Rh1	0.3998	-0.02968	-0.21793
N2	0.352051	0.110661	1.838947
C3	1.498695	0.080947	2.54517
C4	1.52753	0.277115	3.918247
C5	0.326792	0.53029	4.57257
C6	-0.85317	0.568017	3.835862
C7	-0.83318	0.349638	2.454848
C8	-2.1068	0.376243	1.613306
C9	-2.24854	-0.89221	0.772358
C10	-3.36847	-1.72512	0.862218
C11	-3.4883	-2.83831	0.036998
C12	-2.48976	-3.10285	-0.89486
C13	-1.39594	-2.25313	-0.94368
N14	-1.27157	-1.19729	-0.11471
H15	2.407591	-0.0935	1.986049
H16	2.473604	0.23244	4.44513
H17	0.30245	0.698017	5.644935
H18	-1.78937	0.771225	4.335603
H20	-4.15276	-1.4986	1.569855
H21	-4.3593	-3.48151	0.116045
H22	-2.54574	-3.94532	-1.57463
H23	-0.60293	-2.3864	-1.66628
S24	-2.08109	1.870876	0.425255
O25	-3.12853	1.564204	-0.52366
O26	-2.23792	3.024779	1.281739
O27	-0.7002	1.841911	-0.18234
O28	2.173962	1.136371	-0.1544
C29	2.34305	2.314848	-0.53086
O30	1.740827	2.965091	-1.43768
C31	3.471278	3.083496	0.195174
F32	4.656097	2.544326	-0.13824
F33	3.480708	4.377904	-0.11759
F34	3.308581	2.958942	1.52427
O35	0.34164	-0.31546	-2.27914
C36	0.1692	0.587804	-3.15642
O37	0.35621	1.812565	-3.07925
C38	-0.31063	0.015522	-4.51309

F39	-0.67951	0.975912	-5.36008
F40	0.687859	-0.6952	-5.07503
F41	-1.35471	-0.81459	-4.324
H42	1.043634	2.403552	-2.05509
C43	1.886496	-1.92595	-0.30966
H44	2.690519	-1.2769	0.006776
H45	1.268115	-2.43579	0.415751
H46	1.706423	-2.04798	-1.36741
O47	3.141109	-3.46078	-0.35336
V48	3.642831	-4.07842	1.080684
Cl49	5.047394	-5.71837	0.910722
Cl50	4.526384	-2.39546	2.199772
Cl51	1.815903	-4.69965	2.14746
C51	-3.36046	0.627318	2.46938
H52	-4.23713	0.690948	1.822641
H53	-3.51727	-0.1652	3.207802
H54	-3.27211	1.585612	2.98031

Table S219. $[Rh^{IV\text{-}II}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Atom	x	y	z
Rh1	0.178095	-0.28786	-0.18944
N2	0.169759	-0.23377	1.863303
C3	1.324042	-0.40988	2.537521
C4	1.385563	-0.31474	3.920574
C5	0.219566	-0.01797	4.616534
C6	-0.9665	0.161276	3.91031
C7	-0.98411	0.046866	2.517117
C8	-2.26229	0.236823	1.703313
C9	-2.53114	-0.94728	0.775569
C10	-3.74581	-1.64173	0.793905
C11	-3.98366	-2.67473	-0.10592
C12	-3.00291	-3.00353	-1.03626
C13	-1.8123	-2.29422	-1.01444
N14	-1.58185	-1.31074	-0.12176
H15	2.205995	-0.6495	1.958651
H16	2.334033	-0.47438	4.420262
H17	0.22474	0.071985	5.698534
H18	-1.87608	0.394397	4.444355
H20	-4.51139	-1.36637	1.504455
H21	-4.93027	-3.20585	-0.0844
H22	-3.14701	-3.78707	-1.77136
H23	-1.02339	-2.47819	-1.73039

S24	-2.11962	1.813504	0.643054
O25	-3.34775	1.825785	-0.12035
O26	-1.89452	2.867375	1.607823
O27	-0.90714	1.582232	-0.22322
O28	1.998175	0.798869	-0.08582
C29	2.211098	1.992174	-0.38353
O30	1.651483	2.713761	-1.26386
C31	3.33664	2.683293	0.420558
F32	4.513087	2.110634	0.117241
F33	3.410807	3.988092	0.160711
F34	3.108979	2.515697	1.734876
O35	0.087451	-0.49029	-2.26181
C36	0.042071	0.444202	-3.11962
O37	0.329986	1.647146	-3.00775
C38	-0.48336	-0.03001	-4.49835
F39	-0.18246	0.833817	-5.47013
F40	0.03423	-1.2305	-4.81862
F41	-1.82443	-0.1597	-4.43901
H42	0.972458	2.194745	-1.93532
C43	1.308237	-2.16779	-0.22087
H44	2.226309	-1.66188	0.072252
H45	0.807709	-2.77798	0.52234
H46	1.246973	-2.50867	-1.248
O47	2.868007	-3.77103	0.063508
C48	3.675524	-3.37689	0.976275
O49	3.731817	-2.33069	1.61037
C50	4.775553	-4.47141	1.241314
F51	4.246195	-5.704	1.294379
F52	5.683665	-4.44045	0.25069
F53	5.402144	-4.23317	2.398102
C53	-3.47267	0.536491	2.606372
H54	-4.34953	0.736791	1.990098
H55	-3.69006	-0.29266	3.287188
H56	-3.27963	1.438118	3.187799

Table S220. $[Rh^{IV\text{-}II}(DPES)(TFA)_2(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Atom	x	y	z
Rh1	0.196951	-0.03161	-0.13544
N2	0.127658	-0.07811	1.942387
C3	1.284872	-0.21492	2.617585
C4	1.329876	-0.22383	4.005025
C5	0.138646	-0.07717	4.7056

C6	-1.05137	0.068174	3.999193
C7	-1.04649	0.065563	2.599627
C8	-2.3245	0.255709	1.787194
C9	-2.54731	-0.85179	0.757119
C10	-3.72489	-1.6111	0.736125
C11	-3.93333	-2.56429	-0.25368
C12	-2.96525	-2.74202	-1.23616
C13	-1.81228	-1.97583	-1.16484
N14	-1.60161	-1.07759	-0.18461
H15	2.182366	-0.3152	2.023228
H16	2.284641	-0.34525	4.503696
H17	0.128141	-0.07347	5.791937
H18	-1.98062	0.191556	4.536489
H20	-4.48279	-1.45124	1.489229
H21	-4.84761	-3.15085	-0.25943
H22	-3.08717	-3.45356	-2.0451
H23	-1.0296	-2.05505	-1.90747
S24	-2.21818	1.921367	0.856586
O25	-3.43182	1.935009	0.065769
O26	-2.11237	2.904218	1.920362
O27	-0.96083	1.819875	0.057048
O28	1.984509	0.921492	0.100928
C29	2.32463	2.018399	-0.50891
O30	1.853264	2.567832	-1.48226
C31	3.546295	2.647987	0.221696
F32	4.637274	1.852704	0.136619
F33	3.875065	3.843357	-0.29346
F34	3.288071	2.83213	1.538566
O35	0.411194	-0.20853	-2.16724
C36	-0.42897	0.22656	-3.05125
O37	-1.43355	0.902154	-2.94011
C38	-0.09246	-0.39278	-4.43748
F39	-0.71102	0.243206	-5.44416
F40	1.221012	-0.43017	-4.71771
F41	-0.54066	-1.68662	-4.44832
C43	1.204998	-2.03849	-0.09262
H44	2.125597	-1.54041	0.193173
H45	0.666374	-2.59172	0.664728
H46	1.090588	-2.34459	-1.12294
O47	2.698096	-3.73136	0.011428
C48	3.537453	-3.45317	0.928525
O49	3.61797	-2.49396	1.694737

C50	4.646595	-4.55895	1.034215
F51	4.110924	-5.79228	1.173327
F52	5.416978	-4.57512	-0.0747
F53	5.457246	-4.35402	2.086766
C53	-3.554	0.435436	2.694194
H54	-4.43046	0.64416	2.079594
H55	-3.74605	-0.44993	3.310474
H56	-3.40323	1.299408	3.341542

Table S221. [Rh^{III}(DPES)(TFA^{eq})(CH_2TFA^{ax}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	-0.28917	-0.02631	0.012467
N2	-0.16439	0.075768	2.106167
C3	1.028645	-0.01275	2.72529
C4	1.150082	-0.03296	4.106916
C5	-0.00965	0.036568	4.871487
C6	-1.23755	0.14594	4.227267
C7	-1.30204	0.178025	2.830805
C8	-2.61647	0.374291	2.079666
C9	-2.92861	-0.79949	1.153192
C10	-4.15077	-1.47528	1.204857
C11	-4.42122	-2.50887	0.31237
C12	-3.46725	-2.85091	-0.63849
C13	-2.26798	-2.15142	-0.65492
N14	-2.00423	-1.17376	0.232915
H15	1.90166	-0.07597	2.087739
H16	2.133025	-0.10515	4.558282
H17	0.036247	0.014817	5.955991
H18	-2.14362	0.218753	4.811769
H20	-4.89631	-1.18734	1.932065
H21	-5.37365	-3.02817	0.356892
H22	-3.63788	-3.63375	-1.36861
H23	-1.50213	-2.34757	-1.39201
S24	-2.43278	1.969356	1.058258
O25	-3.76753	2.318214	0.636876
O26	-1.72502	2.863864	1.943755
O27	-1.61594	1.531053	-0.14776
O28	1.188038	1.40554	-0.27395
C29	2.38295	1.014253	-0.26865
O30	2.773002	-0.15793	-0.02856
C31	3.46381	2.098074	-0.46864
F32	4.555388	1.587281	-1.04302

F33	3.012749	3.110828	-1.20901
F34	3.806285	2.574497	0.749135
O35	-0.63413	-0.19718	-1.98206
C36	0.312859	-0.28559	-2.86289
O37	1.521929	-0.27019	-2.71106
C38	-0.30629	-0.49215	-4.27284
F39	0.636686	-0.56825	-5.21627
F40	-1.01193	-1.65039	-4.29198
F41	-1.14731	0.505737	-4.5934
H42	1.668074	-0.91352	-0.02515
C43	0.949854	-2.05285	0.118904
H44	1.910632	-2.40547	0.520135
H45	0.191701	-2.37707	0.828705
O46	0.701316	-2.72847	-1.12119
C47	1.718219	-3.39863	-1.68471
O48	2.813741	-3.57112	-1.22093
C49	1.284896	-3.9492	-3.06286
F50	1.558318	-3.05669	-4.02262
F51	1.952206	-5.07804	-3.32223
F52	-0.03509	-4.21778	-3.09225
C52	-3.77754	0.685447	3.038326
H53	-4.67196	0.932874	2.467347
H54	-3.9946	-0.15555	3.704174
H55	-3.52816	1.559807	3.642164

Table S222. $[Rh^{III}(DPES)(TFA^{eq})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Atom	x	y	z
Rh1	-0.56517	-0.21598	-0.16759
N2	-0.43033	0.051301	1.889851
C3	0.764549	0.338469	2.430431
C4	0.89935	0.641777	3.77888
C5	-0.24552	0.661954	4.567986
C6	-1.4801	0.372544	3.991026
C7	-1.56144	0.059969	2.631256
C8	-2.88622	-0.28357	1.946422
C9	-2.8058	-1.63527	1.235397
C10	-3.64585	-2.70206	1.568352
C11	-3.58237	-3.89501	0.855807
C12	-2.67318	-4.00963	-0.19083
C13	-1.85275	-2.92636	-0.46974
N14	-1.91348	-1.77518	0.227211
H15	1.604181	0.349037	1.74917

H16	1.879341	0.868109	4.183279
H17	-0.18594	0.905288	5.624438
H18	-2.37442	0.396398	4.597635
H20	-4.35831	-2.59715	2.374319
H21	-4.24129	-4.71865	1.113376
H22	-2.5913	-4.91307	-0.78452
H23	-1.12747	-2.96837	-1.27233
S24	-3.31592	1.001958	0.617257
O25	-4.27012	0.31662	-0.22889
O26	-3.74021	2.182619	1.327046
O27	-1.99392	1.262264	-0.08261
O28	0.734725	1.346557	-0.26995
C29	1.723223	1.395143	-1.1029
O30	2.028282	0.619201	-1.99468
C31	2.622557	2.620187	-0.78671
F32	1.919532	3.75911	-0.70104
F33	3.228882	2.416477	0.412897
F34	3.57815	2.779132	-1.70673
H35	-0.06163	-1.05671	-2.07363
O36	1.055216	-1.51258	-0.03068
C37	1.399023	-2.08431	-1.10115
O38	0.799037	-1.99921	-2.20144
C39	2.601	-3.04521	-1.00314
F40	3.187653	-3.21542	-2.18577
F41	3.502985	-2.59614	-0.12408
F42	2.144403	-4.24151	-0.57148
C43	-1.14868	-0.20221	-2.39899
H44	-1.13701	-0.90434	-3.24584
H45	-2.17982	-0.12901	-2.05987
O46	-0.76451	1.089529	-2.87305
C47	-0.14332	1.14994	-4.05512
O48	0.054431	0.242255	-4.82151
C49	0.235804	2.615062	-4.35996
F50	0.746801	3.23672	-3.2839
F51	1.130088	2.662974	-5.349
F52	-0.86575	3.288562	-4.74592
C52	-4.07387	-0.21842	2.920605
H53	-5.00187	-0.42809	2.385448
H54	-3.96753	-0.93512	3.74061
H55	-4.15805	0.787568	3.331389

Table S223. [Rh^{III}(DPES)(TFA^{ax})(CH_2TFA^{eq}-H-TFA^{eq})]‡

Atom	x	y	z
Rh1	-0.06254	-0.2911	-0.28516
N2	-0.08421	-0.19025	1.770773
C3	1.054391	-0.42865	2.442313
C4	1.142803	-0.21894	3.811845
C5	0.017621	0.251243	4.481562
C6	-1.16214	0.468289	3.773579
C7	-1.20671	0.232303	2.397125
C8	-2.48391	0.405513	1.568812
C9	-2.77591	-0.87434	0.778985
C10	-3.98181	-1.56992	0.908529
C11	-4.17939	-2.76512	0.224515
C12	-3.15504	-3.27123	-0.56866
C13	-1.98555	-2.53489	-0.67587
N14	-1.81756	-1.36221	-0.04129
H15	1.883634	-0.79828	1.853681
H16	2.076082	-0.41633	4.326698
H17	0.049237	0.442071	5.549844
H18	-2.04253	0.82196	4.291088
H20	-4.76612	-1.17944	1.540671
H21	-5.12046	-3.29738	0.322796
H22	-3.25213	-4.20897	-1.10371
H23	-1.14879	-2.88003	-1.26734
S24	-2.2896	1.850075	0.370343
O25	-3.43369	1.744589	-0.507
O26	-2.1629	3.020897	1.203634
O27	-0.98559	1.557344	-0.34684
O28	1.725057	0.753178	-0.19727
C29	1.992131	1.461803	-1.21181
O30	1.334489	1.508717	-2.2718
C31	3.229808	2.3733	-1.07193
F32	4.207845	1.743223	-0.40246
F33	3.697728	2.744289	-2.26531
F34	2.885691	3.474229	-0.38102
H35	0.0884	-0.12887	-3.5631
H36	0.401841	0.565895	-2.19175
O37	0.969158	-2.04325	-0.1174
C38	1.99618	-2.26603	-0.88894
O39	2.342113	-1.68551	-1.9011
C40	2.829625	-3.45015	-0.33175
F41	3.869023	-3.73417	-1.1191
F42	3.304488	-3.13613	0.896465

F43	2.075475	-4.56144	-0.20883
C44	-0.34784	-0.4907	-2.62108
H45	-0.07747	-1.53953	-2.56294
O46	-1.78103	-0.4273	-2.72421
C47	-2.32457	0.652984	-3.29957
O48	-1.73839	1.58723	-3.77699
C49	-3.85896	0.48666	-3.37723
F50	-4.34752	-0.29088	-2.39519
F51	-4.46514	1.669994	-3.33945
F52	-4.16165	-0.10848	-4.55445
C52	-3.68044	0.822313	2.441903
H53	-4.55585	0.98301	1.81084
H54	-3.91544	0.065426	3.196219
H55	-3.46332	1.769363	2.935747

Rh(PN) complexes in TFAH

A P superscript (e.g. $TFAH^{P}$) refers to an equatorial ligand *trans* to the phosphine in the (PN) ligand, whereas an N superscript refers to an equatorial ligand *trans* to the nitrogen.

Table S224. $Rh^{I}(PN)(TFA^{N})(TFAH^{P})$

Atom	x	y	z
Rh1	0.634194	-0.32947	-0.19454
N2	-0.02531	-0.23643	1.762917
C3	0.595713	0.626492	2.652897
C4	0.196116	0.700342	4.018312
C5	-0.868	-0.12897	4.45452
C6	-1.46429	-0.97677	3.552851
C7	-1.01332	-1.00624	2.217715
C8	0.88489	1.590794	4.882948
H9	-1.19163	-0.08685	5.490796
H10	-2.27806	-1.63289	3.842054
C11	1.662636	1.440454	2.1861
C12	2.318671	2.285336	3.062793
H13	-1.46615	-1.67194	1.493779
P14	2.054694	1.163777	0.428348
O15	-1.03687	-1.71532	-0.65148
C16	0.978697	-0.06144	-3.19937
O17	1.498489	-0.42659	-2.11494
O18	-0.21882	0.185638	-3.47718
C19	1.987396	0.063037	-4.36894
F20	1.483811	0.752537	-5.39851

F21	3.117732	0.681219	-3.9661
F22	2.325165	-1.16594	-4.80744
C23	1.925786	2.363259	4.417717
H24	3.145142	2.893851	2.70961
H25	2.450297	3.035464	5.089865
H26	0.578217	1.646346	5.923998
C27	-3.29439	-2.36315	-1.08763
C28	-2.02489	-1.52619	-1.37502
O29	-2.16009	-0.73896	-2.36982
F30	-3.28224	-2.83179	0.174541
F31	-3.34605	-3.41412	-1.92342
F32	-4.40541	-1.6328	-1.24957
N33	3.740084	0.850991	0.326571
C34	4.263715	-0.43964	0.235163
C35	5.622988	-0.36342	0.373383
C36	5.96197	1.013835	0.56209
C37	4.800163	1.737742	0.535576
H38	3.602312	-1.27472	0.060209
H39	6.308904	-1.19768	0.324558
H40	6.955239	1.425237	0.682434
H41	4.62428	2.800104	0.597958
N42	2.064511	2.761575	-0.2309
C43	2.53453	3.055362	-1.51283
C44	2.103596	4.310289	-1.85335
C45	1.32165	4.809381	-0.76661
C46	1.295846	3.842682	0.203736
H47	2.330565	4.822597	-2.77821
H48	0.844557	5.777788	-0.70167
H49	-1.22784	-0.27604	-2.75179
H50	0.814962	3.826599	1.168516
H51	3.120365	2.33515	-2.0627

Table S225. $Rh^{I}(PN)(TFA^{P})(TFAH^{N})$

Atom	x	y	z
Rh1	0.618781	-0.35428	-0.18667
N2	-0.00405	-0.26411	1.77531
C3	0.606005	0.620351	2.651328
C4	0.196964	0.717617	4.012083
C5	-0.85984	-0.11588	4.457705
C6	-1.44461	-0.98485	3.569063
C7	-0.98953	-1.03364	2.23554
C8	0.864847	1.638915	4.860434

H9	-1.18929	-0.05686	5.490984
H10	-2.25517	-1.64137	3.865999
C11	1.664647	1.439133	2.173794
C12	2.297534	2.318065	3.03388
H13	-1.4375	-1.70584	1.514153
P14	2.071398	1.121619	0.427427
O15	-0.96398	-1.78257	-0.5879
C16	0.894188	0.105331	-3.21447
O17	1.394549	-0.35455	-2.17821
O18	-0.33109	0.344438	-3.48867
C19	1.850248	0.418274	-4.38829
F20	1.500992	1.555555	-5.00357
F21	3.116122	0.540834	-3.95912
F22	1.803885	-0.5839	-5.28462
C23	1.893237	2.421051	4.38363
H24	3.113301	2.935156	2.671006
H25	2.399232	3.11983	5.042656
H26	0.549948	1.713198	5.897817
C27	-3.14407	-2.53818	-1.06926
C28	-1.95741	-1.57604	-1.33083
O29	-2.11989	-0.72403	-2.23408
F30	-3.46094	-2.53206	0.24922
F31	-2.80476	-3.79759	-1.40075
F32	-4.24062	-2.20201	-1.75439
N33	3.75107	0.759807	0.362349
C34	4.232094	-0.54829	0.284188
C35	5.590374	-0.51862	0.449343
C36	5.972087	0.846532	0.642962
C37	4.835948	1.609286	0.59295
H38	3.54473	-1.36163	0.104895
H39	6.247659	-1.37648	0.418186
H40	6.976046	1.22394	0.783841
H41	4.695289	2.676918	0.65345
N42	2.139212	2.70732	-0.26232
C43	2.674525	2.966365	-1.52651
C44	2.213493	4.185192	-1.95002
C45	1.345295	4.695193	-0.93638
C46	1.299742	3.770355	0.073304
H47	2.478985	4.668748	-2.88005
H48	0.826313	5.643883	-0.94406
H49	-1.06894	-0.08391	-2.80783
H50	0.758516	3.772415	1.006133

H51	3.332075	2.25476	-2.00121

Table S226. $Rh^{III}(PN)(TFA)_3(TFAH^P)$

Atom	x	y	z
Rh1	0.415024	-0.00619	-0.20156
N2	-0.17428	-0.10962	1.820912
C3	0.691586	0.395701	2.762872
C4	0.435346	0.233582	4.153745
C5	-0.76267	-0.41737	4.542233
C6	-1.6202	-0.87793	3.575457
C7	-1.28429	-0.71494	2.21458
C8	1.387008	0.716236	5.08846
H9	-0.98233	-0.54562	5.598422
H10	-2.54729	-1.38067	3.826544
C11	1.867377	1.078456	2.353394
C12	2.787723	1.514785	3.290277
H13	-1.9217	-1.10169	1.430747
P14	2.06667	1.264973	0.574257
O15	-1.41116	-1.24082	-0.57904
C16	0.955088	0.092489	-3.23102
O17	1.381514	0.188592	-2.03949
O18	-0.14856	-0.23964	-3.67977
C19	2.043005	0.498332	-4.26327
F20	1.645392	0.283846	-5.5181
F21	2.320069	1.819831	-4.1332
F22	3.180606	-0.18171	-4.05152
C23	2.545734	1.331521	4.668365
H24	3.701632	2.001595	2.961863
H25	3.274734	1.681858	5.39191
H26	1.187854	0.581023	6.147933
C27	-3.32697	-2.55825	-1.09718
C28	-2.13208	-1.65664	-1.49273
O29	-2.03552	-1.47698	-2.7498
F30	-3.66164	-2.35886	0.193393
F31	-2.98494	-3.84707	-1.24482
F32	-4.40085	-2.30635	-1.85116
N33	3.670615	0.912614	0.166275
C34	4.239907	-0.36706	0.084039
C35	5.589572	-0.21936	-0.05551
C36	5.885324	1.181968	-0.05546
C37	4.710675	1.861497	0.086862
H38	3.618365	-1.24417	0.140789

H39	6.297286	-1.02984	-0.1603
H40	6.859468	1.638334	-0.1667
H41	4.495834	2.917488	0.103549
N42	1.978047	2.910131	0.215645
C43	2.060453	3.424547	-1.08874
C44	1.995851	4.78535	-1.00679
C45	1.86027	5.139164	0.375377
C46	1.844202	3.986826	1.105881
H47	2.029269	5.463873	-1.84769
H48	1.767095	6.137031	0.781094
H49	-1.18043	-0.9158	-3.05082
H50	1.707345	3.817155	2.160277
H51	2.153961	2.762818	-1.93516
O53	1.45552	-1.73825	0.232515
C54	1.356295	-2.72227	-0.61527
O55	0.785113	-2.76984	-1.68874
C56	2.105026	-3.97129	-0.07481
F57	2.033585	-4.99474	-0.92904
F58	3.414335	-3.69255	0.133145
F59	1.582109	-4.36862	1.104163
O60	-0.73078	1.595829	-0.75941
C61	-1.18962	2.461517	0.086364
O62	-0.97864	2.554841	1.286547
C63	-2.10899	3.491153	-0.62575
F64	-2.64623	4.347504	0.253125
F65	-1.41001	4.203058	-1.53072
F66	-3.11664	2.870596	-1.27144

Table S227. $Rh^{III}(PN)(TFA)_3(TFAH^{ax})$

Atom	x	y	z
Rh1	0.460383	0.007876	-0.1772
N2	-0.23728	-0.08445	1.773183
C3	0.545232	0.41889	2.785806
C4	0.170788	0.225493	4.144988
C5	-1.05911	-0.42753	4.414297
C6	-1.83604	-0.86903	3.371953
C7	-1.38205	-0.69394	2.047908
C8	1.041988	0.682282	5.166755
H9	-1.36881	-0.57275	5.445302
H10	-2.78351	-1.36925	3.53691
C11	1.747185	1.114742	2.478659
C12	2.585707	1.515357	3.504379

H13	-1.93032	-1.07784	1.19408
P14	2.036115	1.401094	0.711395
O15	-0.97017	-1.44849	-0.65816
C16	0.91662	0.533289	-3.16396
O17	1.285086	-0.16276	-2.10145
O18	0.637992	1.707761	-3.20507
C19	1.011887	-0.27547	-4.48335
F20	0.045358	0.070479	-5.32958
F21	2.203636	-0.00677	-5.06566
F22	0.956289	-1.60659	-4.27927
C23	2.233406	1.296692	4.854071
H24	3.531701	1.994556	3.273447
H25	2.905081	1.623307	5.641301
H26	0.755548	0.526733	6.202989
C27	-2.88737	-2.39616	-1.60919
C28	-1.66589	-1.44577	-1.75716
O29	-1.48789	-0.84842	-2.80101
F30	-2.48671	-3.67476	-1.44918
F31	-3.69689	-2.34067	-2.66813
F32	-3.6167	-2.06213	-0.51155
N33	3.689035	0.996571	0.515109
C34	4.321709	-0.14614	1.020421
C35	5.541113	-0.26223	0.41192
C36	5.672874	0.821745	-0.51397
C37	4.531101	1.569632	-0.44727
H38	3.837311	-0.7678	1.755847
H39	6.273601	-1.03088	0.616834
H40	6.524272	1.033716	-1.14556
H41	4.234048	2.464514	-0.97169
N42	2.047855	3.050909	0.370347
C43	1.558192	3.624672	-0.81743
C44	1.829678	4.961993	-0.77364
C45	2.49789	5.242591	0.461665
C46	2.626876	4.068315	1.143929
H47	1.568631	5.673992	-1.54385
H48	2.834739	6.208949	0.811475
H49	1.653125	-1.53138	-2.05438
H50	3.053042	3.86063	2.111122
H51	1.081237	3.013397	-1.57242
O53	1.679217	-1.66279	0.366402
C54	2.079596	-2.51469	-0.44945
O55	2.03181	-2.47143	-1.72329

C56	2.695282	-3.80369	0.139462
F57	3.369273	-3.51628	1.2646
F58	1.708847	-4.6621	0.441399
F59	3.528079	-4.38623	-0.72399
O60	-0.87262	1.420742	-0.69438
C61	-1.22111	2.369322	0.119308
O62	-0.80447	2.615536	1.240457
C63	-2.29826	3.276392	-0.53678
F64	-2.77136	4.162473	0.350393
F65	-1.76717	3.955886	-1.56819
F66	-3.33271	2.54973	-0.99439

Table S228. $[Rh^{III}(PN)(TFA)_2(TFAH^{ax})(TFAH^{p})]^+$

Atom	x	y	z
Rh1	0.368909	-0.11076	-0.22051
N2	-0.24022	-0.25866	1.76189
C3	0.562	0.275505	2.744331
C4	0.237845	0.09956	4.118624
C5	-0.95449	-0.59515	4.444172
C6	-1.74449	-1.09168	3.435432
C7	-1.34585	-0.91383	2.096509
C8	1.121956	0.616222	5.10218
H9	-1.22651	-0.73015	5.486992
H10	-2.66303	-1.62961	3.639683
C11	1.736855	0.992137	2.39389
C12	2.592783	1.458251	3.379851
H13	-1.93063	-1.32514	1.285645
P14	1.992424	1.201206	0.632756
O15	-1.2899	-1.51007	-0.84369
C16	0.684581	0.315184	-3.27231
O17	1.234245	-0.02936	-2.14519
O18	-0.49705	0.490594	-3.5278
C19	1.74777	0.544492	-4.37869
F20	1.191829	0.728186	-5.56612
F21	2.480004	1.634983	-4.0605
F22	2.57926	-0.51371	-4.43423
C23	2.280892	1.269228	4.743077
H24	3.509305	1.972664	3.106901
H25	2.957337	1.64522	5.503307
H26	0.871467	0.477623	6.149956
C27	-3.537	-2.24546	-1.15039
C28	-2.32719	-1.34485	-1.50277

O29	-2.5492	-0.51439	-2.45312
F30	-3.84044	-2.0461	0.153763
F31	-3.19598	-3.5276	-1.31324
F32	-4.60601	-1.96891	-1.88381
N33	3.588941	0.699636	0.350312
C34	4.205991	-0.4151	0.951654
C35	5.358328	-0.68072	0.268678
C36	5.467175	0.26775	-0.80145
C37	4.382066	1.091281	-0.74614
H38	3.776613	-0.88285	1.822985
H39	6.070286	-1.45549	0.517534
H40	6.274606	0.342962	-1.51631
H41	4.103329	1.937849	-1.35338
N42	1.970732	2.815223	0.188572
C43	1.853837	3.294707	-1.1323
C44	1.91068	4.656336	-1.0918
C45	2.052944	5.053909	0.276975
C46	2.084958	3.929079	1.044161
H47	1.85013	5.310176	-1.95053
H48	2.108891	6.066487	0.651363
H49	2.250349	-1.25867	-2.03408
H50	2.126899	3.804742	2.112932
H51	1.769552	2.613776	-1.96186
O53	1.517273	-1.86199	0.192024
C54	2.36416	-2.41759	-0.52527
O55	2.73443	-2.08493	-1.71318
C56	3.044474	-3.69611	0.018041
F57	4.252902	-3.8556	-0.51673
F58	3.15658	-3.60891	1.348767
F59	2.277014	-4.74841	-0.28911
O60	-0.87933	1.378883	-0.69834
C61	-1.20804	2.328825	0.13925
O62	-0.79882	2.507175	1.270175
C63	-2.24105	3.287629	-0.51364
F64	-2.64973	4.203975	0.36247
F65	-1.68474	3.910142	-1.56661
F66	-3.31002	2.592893	-0.94409
H66	-1.71371	0.00142	-2.7463

Table S229. [$Rh^{III}(PN)(TFA)_2(TFAH^{eq})_2$]$^+$

Atom	x	y	z
Rh1	0.471711	0.014777	-0.11173

N2	0.25677	-0.72141	1.797012
C3	1.352369	-0.72298	2.627748
C4	1.283347	-1.34001	3.90846
C5	0.049179	-1.9057	4.314758
C6	-1.03039	-1.86664	3.463278
C7	-0.88326	-1.27386	2.195549
C8	2.454488	-1.38011	4.711992
H9	-0.02747	-2.37336	5.292028
H10	-1.98784	-2.2957	3.735174
C11	2.572675	-0.13423	2.199846
C12	3.704336	-0.22428	2.994053
H13	-1.69871	-1.26609	1.482709
P14	2.504108	0.679014	0.60024
O15	-1.53472	-0.78574	-0.79212
C16	0.475345	0.705479	-3.17459
O17	0.805067	0.945197	-1.99479
O18	0.051413	-0.38348	-3.67406
C19	0.518085	1.903835	-4.15553
F20	-0.66759	2.530138	-4.09074
F21	1.479709	2.761507	-3.78841
F22	0.738823	1.501156	-5.40203
C23	3.642094	-0.84868	4.259228
H24	4.647956	0.184171	2.644481
H25	4.536284	-0.9042	4.871076
H26	2.400475	-1.85362	5.687825
C27	-3.62947	-0.89444	-1.9421
C28	-2.48175	-0.12838	-1.24154
O29	-2.62771	1.15575	-1.19517
F30	-4.58822	-0.07515	-2.35918
F31	-4.14057	-1.77369	-1.06854
F32	-3.12152	-1.55917	-2.98638
N33	2.691178	2.335796	0.740168
C34	3.330194	3.032023	1.784384
C35	3.342853	4.355106	1.460685
C36	2.700815	4.508542	0.188585
C37	2.305008	3.27585	-0.23963
H38	3.674413	2.516092	2.665279
H39	3.755543	5.144234	2.073515
H40	2.54299	5.434943	-0.34573
H41	1.802136	2.957272	-1.13863
N42	3.854946	0.173487	-0.26883
C43	4.266536	-1.1645	-0.4412

C44	5.233422	-1.18644	-1.40017
C45	5.433041	0.15905	-1.86341
C46	4.584022	0.973302	-1.17876
H47	5.763946	-2.06748	-1.73366
H48	6.147377	0.484606	-2.60684
H49	-1.87915	1.576883	-0.66091
H50	4.437452	2.041076	-1.21133
H51	3.81502	-1.95981	0.12745
O53	1.306907	-1.84876	-0.42383
C54	1.009602	-2.65714	-1.36658
O55	0.415298	-2.4505	-2.43187
C56	1.468946	-4.1066	-1.05546
F57	1.266354	-4.91721	-2.08652
F58	2.779589	-4.11661	-0.74213
F59	0.780337	-4.56379	0.00683
O60	-0.54306	1.771885	0.237577
C61	-0.48474	2.422927	1.382728
O62	0.176586	2.131273	2.354711
C63	-1.37395	3.693205	1.350935
F64	-1.52476	4.198417	2.570704
F65	-0.81749	4.619695	0.554987
F66	-2.5934	3.386913	0.853408
H66	0.149427	-1.24538	-3.03919

Table S230. $Rh^{III}(PN)(TFA)_2(TFAH^{P})(CH_3{}^{ax})$

Atom	x	y	z
Rh1	0.593069	-0.24585	-0.02198
N2	-0.02305	-0.24562	1.969433
C3	0.755936	0.403726	2.89947
C4	0.417705	0.377469	4.282011
C5	-0.76346	-0.3033	4.671199
C6	-1.52924	-0.91985	3.713815
C7	-1.11916	-0.87551	2.364887
C8	1.270957	1.029206	5.208364
H9	-1.04553	-0.32647	5.720195
H10	-2.44278	-1.44694	3.965
C11	1.913523	1.111239	2.476302
C12	2.727145	1.726917	3.410653
H13	-1.69429	-1.36577	1.590543
P14	2.162779	1.126664	0.682414
O15	-1.13791	-1.57763	-0.516
C16	1.018168	0.006461	-3.04148

O17	1.512967	-0.26405	-1.90654
O18	-0.16236	0.098205	-3.41349
C19	2.110481	0.209147	-4.12472
F20	1.601038	0.642073	-5.27984
F21	3.03131	1.107523	-3.70921
F22	2.749373	-0.95559	-4.35139
C23	2.407776	1.680657	4.784757
H24	3.620364	2.251986	3.08927
H25	3.058479	2.170566	5.502034
H26	1.010055	1.002739	6.262942
C27	-3.38465	-2.20653	-0.93081
C28	-2.10046	-1.41841	-1.28334
O29	-2.18818	-0.72416	-2.34562
F30	-3.68214	-2.02182	0.375091
F31	-3.16891	-3.51932	-1.12376
F32	-4.43656	-1.83164	-1.65637
N33	3.802795	0.842415	0.319641
C34	4.368346	-0.33255	-0.18852
C35	5.726308	-0.18572	-0.19585
C36	6.030487	1.113769	0.321761
C37	4.849996	1.728372	0.627025
H38	3.739359	-1.1332	-0.53234
H39	6.433112	-0.91956	-0.55713
H40	7.012191	1.553767	0.432746
H41	4.640869	2.725668	0.97984
N42	2.081224	2.766615	0.244155
C43	2.461736	3.243704	-1.02123
C44	2.122223	4.563592	-1.0943
C45	1.494786	4.925168	0.141847
C46	1.464971	3.817027	0.938583
H47	2.300475	5.209828	-1.9426
H48	1.103966	5.897114	0.40923
H49	-1.26319	-0.27905	-2.67951
H50	1.022526	3.654073	1.906409
H51	2.931379	2.588704	-1.73798
O60	-0.71319	1.373149	-0.71595
C61	-1.29164	2.177363	0.096039
O62	-1.16301	2.286596	1.315384
C63	-2.27359	3.131169	-0.63918
F64	-2.96583	3.898723	0.218916
F65	-1.60564	3.951847	-1.47658
F66	-3.16692	2.432237	-1.37341

C59	1.601787	-2.00937	0.444019
H60	2.05536	-2.38245	-0.47717
H61	2.352966	-1.93202	1.233961
H62	0.808717	-2.69275	0.760066

Table S231. $Rh^{III}(PN)(TFA)_2(TFAH^N)(CH_3^{ax})$

Atom	x	y	z
Rh1	0.488384	-0.27848	-0.06001
N2	-0.17307	-0.03005	1.878082
C3	0.684574	0.519497	2.805759
C4	0.335652	0.561909	4.186167
C5	-0.94701	0.089343	4.564145
C6	-1.80203	-0.38639	3.601063
C7	-1.37533	-0.44342	2.257101
C8	1.277347	1.081023	5.111497
H9	-1.23852	0.117527	5.609994
H10	-2.79667	-0.74123	3.846043
C11	1.920308	1.06896	2.3701
C12	2.810716	1.568731	3.303371
H13	-2.00223	-0.86275	1.481543
P14	2.107454	1.121807	0.556461
O15	-1.1394	-1.68689	-0.30516
C16	0.994863	-0.19015	-3.10806
O17	1.388577	-0.51173	-1.96915
O18	-0.12993	-0.40707	-3.65959
C19	2.060941	0.393205	-4.06176
F20	1.526845	1.155695	-5.01168
F21	2.967567	1.112704	-3.37974
F22	2.712536	-0.6344	-4.65077
C23	2.496483	1.555936	4.68075
H24	3.761179	1.978348	2.978146
H25	3.215284	1.944884	5.394842
H26	1.017522	1.099097	6.166064
C27	-3.25056	-2.59968	-0.77977
C28	-1.98203	-1.82983	-1.23407
O29	-1.9462	-1.47283	-2.42546
F30	-3.79499	-1.98665	0.302212
F31	-2.9309	-3.856	-0.41449
F32	-4.18467	-2.66025	-1.72929
N33	3.726416	0.833587	0.13159
C34	4.227495	-0.31393	-0.49601
C35	5.588072	-0.21361	-0.54738

C36	5.960931	1.027139	0.061556
C37	4.818009	1.654376	0.467554
H38	3.552494	-1.0596	-0.87676
H39	6.252252	-0.93944	-0.99515
H40	6.962313	1.421731	0.166422
H41	4.660507	2.626444	0.906497
N42	2.027256	2.797071	0.245943
C43	2.513439	3.432719	-0.90617
C44	2.068616	4.722582	-0.90085
C45	1.2528	4.901722	0.261513
C46	1.226054	3.717031	0.939734
H47	2.288165	5.462241	-1.6578
H48	0.745764	5.80735	0.563988
H49	-0.87627	-0.85708	-3.02904
H50	0.726996	3.440425	1.853986
H51	3.095245	2.887103	-1.63014
O60	-0.945	1.293109	-0.61636
C61	-0.74815	2.110452	-1.58171
O62	0.175857	2.156955	-2.39449
C63	-1.87677	3.173595	-1.68032
F64	-3.07816	2.584406	-1.86382
F65	-1.95158	3.899051	-0.53965
F66	-1.68062	4.029002	-2.69329
C59	1.550042	-1.95707	0.592999
H60	1.919321	-2.46595	-0.30006
H61	2.376818	-1.75809	1.279649
H62	0.800681	-2.58104	1.084893

Table S232. $Rh^{III}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3^{ax})$

Atom	x	y	z
Rh1	-0.21927	1.381859	2.051802
N2	1.537925	2.514969	1.94117
C3	2.740379	1.860068	1.804315
C4	3.972923	2.567276	1.916901
C5	3.921537	3.970865	2.111074
C6	2.702239	4.597324	2.203597
C7	1.521674	3.828525	2.131849
C8	5.18692	1.838191	1.839589
H9	4.848456	4.532132	2.190145
H10	2.621831	5.668067	2.35432
C11	2.741547	0.460423	1.55782
C12	3.948019	-0.21428	1.503979

H13	0.542963	4.272965	2.272747
P14	1.086485	-0.28607	1.276442
O15	-1.17821	3.123377	2.834144
C16	-2.33041	-0.64777	1.742646
O17	-2.01014	0.429853	2.36433
O18	-1.65337	-1.31588	0.968094
C19	-3.77045	-1.10107	2.095264
F20	-4.15806	-2.13437	1.337098
F21	-3.8258	-1.4887	3.388185
F22	-4.65019	-0.09921	1.923027
C23	5.172894	0.473577	1.657303
H24	3.958141	-1.28673	1.339876
H25	6.104627	-0.08153	1.61302
H26	6.126349	2.375678	1.934096
C27	-2.75402	4.688807	3.576342
C28	-2.36806	3.518921	2.633626
O29	-3.22024	3.14051	1.817732
F30	-1.86306	5.69954	3.433361
F31	-2.71901	4.291208	4.861958
F32	-3.97178	5.172321	3.318067
N33	1.153959	-1.85234	1.940929
C34	0.580142	-2.25414	3.148554
C35	0.964407	-3.54167	3.400227
C36	1.798773	-3.96631	2.319294
C37	1.903259	-2.92597	1.438034
H38	-0.06487	-1.5884	3.695926
H39	0.663392	-4.12986	4.255728
H40	2.250828	-4.94062	2.193378
H41	2.383247	-2.85837	0.474786
N42	1.187875	-0.63936	-0.39671
C43	0.390358	-1.54765	-1.1076
C44	0.743101	-1.48195	-2.42588
C45	1.769548	-0.49495	-2.56033
C46	2.020899	0.01425	-1.31905
H47	0.307412	-2.07579	-3.2174
H48	2.263874	-0.1915	-3.47292
H49	2.713237	0.776044	-1.00303
H50	-0.35721	-2.1286	-0.59611
O51	-0.71569	1.941133	-0.17888
C52	-1.78676	1.812891	-0.77336
O53	-2.98037	1.865801	-0.29003
C54	-1.7871	1.553028	-2.29921

F55	-2.64555	2.382784	-2.91612
F56	-0.56958	1.745977	-2.81721
F57	-2.16728	0.289025	-2.54683
C58	0.251171	1.018142	4.027995
H59	-0.57327	0.437192	4.443374
H60	1.206067	0.507638	4.171692
H61	0.272953	2.010345	4.481936
H62	-3.01453	2.26414	0.681813

Table S233. $[Rh^{III}(PN)(TFA^{ax})(TFAH^{eq})_2(CH_3^{ax})]^+$

Atom	x	y	z
Rh1	0.578711	-0.19464	0.133377
N2	0.024222	-0.19775	2.119272
C3	0.843966	0.406907	3.045102
C4	0.524253	0.367875	4.432801
C5	-0.66982	-0.28289	4.830048
C6	-1.47047	-0.86672	3.877051
C7	-1.08282	-0.81153	2.525424
C8	1.41641	0.972979	5.355693
H9	-0.93543	-0.31728	5.882609
H10	-2.38966	-1.37797	4.139037
C11	2.023886	1.072468	2.615724
C12	2.873662	1.64456	3.54842
H13	-1.67695	-1.29199	1.758319
P14	2.244317	1.121818	0.824254
O15	-1.10926	-1.56682	-0.42884
C16	1.205138	0.485097	-2.81788
O17	1.302211	-0.32193	-1.88059
O18	0.495747	1.558088	-2.87165
C19	2.085962	0.257972	-4.06784
F20	1.470636	0.672116	-5.17207
F21	3.213972	0.97337	-3.89314
F22	2.401413	-1.03046	-4.18478
C23	2.571032	1.5883	4.925445
H24	3.782735	2.140745	3.225609
H25	3.250261	2.04031	5.640476
H26	1.173614	0.937786	6.413471
C27	-3.01839	-2.58116	-1.43871
C28	-2.0984	-1.37467	-1.14175
O29	-2.48643	-0.25336	-1.65868
F30	-3.52237	-3.00585	-0.2672
F31	-2.29202	-3.5627	-1.98183

F32	-4.01477	-2.2588	-2.25596
N33	3.829607	0.784117	0.35461
C34	4.311444	-0.36983	-0.29185
C35	5.667477	-0.27079	-0.38544
C36	6.064524	0.967743	0.215879
C37	4.941349	1.600709	0.657326
H38	3.633075	-1.12454	-0.64575
H39	6.317034	-0.99795	-0.85196
H40	7.071411	1.35405	0.293266
H41	4.806868	2.571124	1.108079
N42	2.174634	2.772426	0.4345
C43	2.57623	3.30123	-0.80989
C44	2.159325	4.598351	-0.87284
C45	1.46372	4.898532	0.3443
C46	1.470937	3.777001	1.121496
H47	2.34539	5.277867	-1.69287
H48	1.022756	5.846882	0.618266
H49	-1.89091	0.504852	-1.34951
H50	1.036912	3.586824	2.08903
H51	3.153138	2.708325	-1.5028
O60	-0.80796	1.493907	-0.70031
C61	-1.34723	2.408651	0.095842
O62	-1.335	2.394198	1.305574
C63	-2.06635	3.525503	-0.69886
F64	-2.52504	4.482167	0.100802
F65	-1.21974	4.071295	-1.59531
F66	-3.10007	2.984753	-1.3776
H66	-0.04952	1.70647	-2.01496
C60	1.568297	-1.95539	0.581196
H61	1.924888	-2.34476	-0.37376
H62	2.382094	-1.86038	1.300489
H63	0.783473	-2.60226	0.97733

Table S234. [Rh^{III}(PN)(TFA^{N})($TFAH^{ax}$)($TFAH^{P}$)(CH_3^{ax})]$^{+}$

Atom	x	y	z
Rh1	0.991944	0.328873	0.507601
N2	-0.22288	-1.36052	0.584514
C3	-0.70178	-1.77224	1.809582
C4	-1.45967	-2.97286	1.929118
C5	-1.74209	-3.70781	0.750171
C6	-1.27587	-3.25104	-0.45991
C7	-0.50672	-2.07191	-0.50254

C8	-1.89418	-3.38173	3.217475
H9	-2.32314	-4.62318	0.817431
H10	-1.47333	-3.78195	-1.38422
C11	-0.43982	-0.99085	2.968795
C12	-0.87294	-1.42703	4.209971
H13	-0.0986	-1.70776	-1.43698
P14	0.431409	0.557574	2.642582
O15	1.37405	-0.07488	-1.66771
C16	2.206279	3.05741	0.059052
O17	2.311988	1.960415	0.668856
O18	1.464047	3.330618	-0.92024
C19	3.06548	4.206519	0.649766
F20	2.370324	4.754399	1.674656
F21	4.227443	3.749125	1.123768
F22	3.30074	5.151281	-0.25749
C23	-1.59625	-2.63309	4.335228
H24	-0.65426	-0.84231	5.097774
H25	-1.92399	-2.95993	5.316557
H26	-2.46403	-4.30225	3.307113
C27	1.416279	-0.3403	-4.03178
C28	1.378959	0.522223	-2.74735
O29	1.367571	1.792274	-2.96186
F30	0.479142	-1.30355	-3.92361
F31	2.617688	-0.92223	-4.12645
F32	1.178423	0.373238	-5.12551
N33	1.574437	0.91234	3.825567
C34	2.971781	0.773352	3.738441
C35	3.499916	1.010481	4.972361
C36	2.420418	1.300464	5.869551
C37	1.256497	1.239354	5.162996
H38	3.443992	0.56689	2.79529
H39	4.553631	1.003098	5.213494
H40	2.502663	1.54969	6.918553
H41	0.237787	1.44355	5.452214
N42	-0.71498	1.772066	2.953581
C43	-0.38983	3.142201	2.97299
C44	-1.55414	3.85397	2.938555
C45	-2.64012	2.919872	2.873842
C46	-2.11095	1.660368	2.867236
H47	-1.63277	4.931748	2.975067
H48	-3.69449	3.157523	2.853528
H49	-2.58866	0.695145	2.82525

H50	0.638138	3.465315	3.03015
O51	-1.00023	1.418631	-0.21088
C52	-1.64044	2.421729	-0.49872
O53	-1.17812	3.609752	-0.76711
C54	-3.17748	2.342913	-0.65273
F55	-3.77451	3.425133	-0.14905
F56	-3.46754	2.249815	-1.96021
F57	-3.64648	1.254117	-0.03158
C58	2.596313	-0.91144	0.868338
H59	3.487933	-0.28416	0.841159
H60	2.529028	-1.46732	1.804264
H61	2.582731	-1.59463	0.016802
H62	-0.18078	3.605578	-0.76043
H63	1.390949	2.349528	-2.10609

Table S235. $[Rh^{III}(PN)(TFA^{P})(TFAH^{ax})(TFAH^{N})(CH_3^{ax})]^+$

Atom	x	y	z
Rh1	-0.48574	0.236128	1.908048
N2	0.433927	-1.05539	0.583182
C3	-0.24508	-2.18597	0.17592
C4	0.396593	-3.16223	-0.63997
C5	1.728823	-2.91871	-1.05693
C6	2.363862	-1.76636	-0.65837
C7	1.68618	-0.85814	0.177079
C8	-0.31857	-4.33766	-0.99019
H9	2.233402	-3.6477	-1.68385
H10	3.38203	-1.54356	-0.95635
C11	-1.59467	-2.38702	0.576922
C12	-2.25502	-3.55293	0.225785
H13	2.173885	0.037401	0.541837
P14	-2.30386	-1.01924	1.519716
O15	1.398783	1.319688	2.130279
C16	-1.87181	2.493093	3.669106
O17	-1.60261	1.31952	3.374378
O18	-1.31811	3.573365	3.262788
C19	-3.06649	2.703734	4.631545
F20	-3.06833	3.921561	5.160269
F21	-4.20261	2.529072	3.924571
F22	-3.02546	1.790685	5.605815
C23	-1.61042	-4.53658	-0.55529
H24	-3.27666	-3.71606	0.554688
H25	-2.14319	-5.44452	-0.81759

H26	0.176973	-5.08449	-1.60362
C27	3.099286	2.9081	1.720807
C28	1.606738	2.539713	1.931449
O29	0.758313	3.47385	1.868595
F30	3.61323	2.108579	0.756563
F31	3.782365	2.696649	2.852174
F32	3.250008	4.174308	1.342193
N33	-3.2855	-1.5625	2.77939
C34	-2.95906	-1.65702	4.1436
C35	-3.97743	-2.30041	4.781882
C36	-4.97316	-2.6309	3.806015
C37	-4.54304	-2.17805	2.594305
H38	-2.05388	-1.21959	4.523377
H39	-4.02421	-2.49918	5.843382
H40	-5.91504	-3.12929	3.989064
H41	-5.01644	-2.18063	1.625316
N42	-3.47252	-0.34198	0.497383
C43	-4.34479	0.683815	0.905466
C44	-5.00106	1.1447	-0.19885
C45	-4.52423	0.410557	-1.33313
C46	-3.58392	-0.47618	-0.89536
H47	-5.75959	1.915147	-0.20224
H48	-4.85039	0.523124	-2.35747
H49	-2.98937	-1.19699	-1.43196
H50	-4.42363	0.959823	1.945613
O51	-1.0123	1.606054	-0.01954
C52	-0.88024	2.539033	-0.79868
O53	-0.3035	3.689038	-0.57472
C54	-1.44632	2.444588	-2.23779
F55	-0.72675	3.172814	-3.09278
F56	-1.42995	1.165357	-2.63925
F57	-2.71205	2.886138	-2.24262
C58	0.251241	-0.95663	3.41564
H59	-0.05583	-0.49413	4.354444
H60	-0.08206	-1.99308	3.353633
H61	1.332865	-0.8876	3.293635
H62	0.077705	3.724342	0.344993
H63	-0.48188	3.436757	2.659605

Table S236. $Rh^{III}(PN)(TFA^{ax})_2(TFAH^{p})(CH_3{}^{N})$

Atom	x	y	z
Rh1	0.524387	-0.19066	-0.04709

N2	-0.05012	-0.12977	2.174157
C3	0.844321	0.4923	3.000467
C4	0.690804	0.460198	4.417118
C5	-0.44521	-0.20768	4.943507
C6	-1.34063	-0.79853	4.086443
C7	-1.09669	-0.74096	2.694897
C8	1.671081	1.080457	5.23255
H9	-0.59008	-0.24386	6.019644
H10	-2.22185	-1.31423	4.452481
C11	1.96065	1.178827	2.439169
C12	2.90804	1.755297	3.26751
H13	-1.77492	-1.20734	1.987027
P14	2.085585	1.204779	0.628812
O15	-1.42369	-1.32522	-0.35352
C23	2.762482	1.705432	4.671204
H24	3.774138	2.248783	2.836441
H25	3.515162	2.166312	5.303055
H26	1.549858	1.047329	6.311813
C27	-3.33706	-1.89132	-1.6908
C28	-1.84434	-1.98813	-1.30252
O29	-1.18153	-2.82547	-2.02505
F30	-3.88418	-0.78163	-1.19223
F31	-3.98904	-2.95707	-1.18448
F32	-3.48549	-1.89243	-3.02097
N33	3.731257	0.949011	0.243959
C34	4.359757	-0.30016	0.184502
C35	5.708768	-0.0958	0.096851
C36	5.940517	1.315255	0.111624
C37	4.728227	1.939028	0.212764
H38	3.780587	-1.20561	0.237638
H39	6.455146	-0.87447	0.022395
H40	6.896143	1.81637	0.037837
H41	4.466119	2.98448	0.222632
N42	1.933551	2.837216	0.180503
C43	2.106938	3.303141	-1.12951
C44	1.854217	4.645407	-1.1412
C45	1.496804	5.033328	0.190026
C46	1.541798	3.919078	0.97865
H47	1.913098	5.287115	-2.00925
H48	1.224385	6.024681	0.524433
H49	-0.24361	-3.00439	-1.59975
H50	1.293692	3.776227	2.016542

H51	2.407802	2.629905	-1.91678
O53	1.651004	-1.87126	0.539173
C54	1.602274	-3.0348	0.033731
O55	0.945857	-3.4823	-0.91908
C56	2.54645	-4.02748	0.764711
F57	2.466035	-5.26155	0.261861
F58	3.829558	-3.61388	0.656154
F59	2.241193	-4.0833	2.075433
O60	-0.6572	1.319425	-0.74028
C61	-1.28322	2.134675	0.045803
O62	-1.137	2.334758	1.241912
C63	-2.34455	2.937882	-0.75484
F64	-3.04926	3.749124	0.04622
F65	-1.75653	3.696163	-1.70221
F66	-3.21163	2.106608	-1.36989
C59	1.212162	-0.28235	-1.99788
H60	1.068716	0.69221	-2.4671
H61	2.261854	-0.58464	-2.02703
H62	0.600658	-1.02506	-2.51545

Table S237. $[Rh^{II}(PN)(TFA^{N})(TFAH^{P})]^{+}$

Atom	x	y	z
Rh1	0.535462	-0.1903	-0.22385
N2	-0.19627	-0.01818	1.750147
C3	0.533622	0.725004	2.657035
C4	0.144712	0.789813	4.026262
C5	-1.02425	0.093633	4.42539
C6	-1.73797	-0.62375	3.494282
C7	-1.28665	-0.66284	2.161291
C8	0.943899	1.536898	4.930954
H9	-1.34014	0.132809	5.463988
H10	-2.63563	-1.16978	3.760838
C11	1.692861	1.428901	2.225528
C12	2.452395	2.140395	3.140804
H13	-1.8153	-1.2399	1.412263
P14	2.067573	1.272282	0.463809
O15	-1.10709	-1.5834	-0.68253
C16	0.997439	0.00426	-3.11128
O17	1.528156	-0.40597	-2.02554
O18	-0.1759	0.367842	-3.29065
C19	1.997929	0.069056	-4.29343
F20	1.38763	0.391965	-5.4296

F21	2.9359	1.005834	-4.02501
F22	2.61365	-1.11106	-4.44244
C23	2.077207	2.191493	4.500555
H24	3.347739	2.660668	2.815195
H25	2.685721	2.751926	5.202424
H26	0.647652	1.57802	5.97513
C27	-3.17728	-2.62787	-1.21158
C28	-2.03137	-1.6318	-1.50978
O29	-2.17059	-0.95406	-2.58643
F30	-3.61876	-2.39744	0.04392
F31	-2.70046	-3.87534	-1.27314
F32	-4.19166	-2.49358	-2.05597
N33	3.674867	0.874348	0.192557
C34	4.146269	-0.43925	0.012493
C35	5.506376	-0.4168	0.106578
C36	5.909253	0.935561	0.359604
C37	4.787359	1.709567	0.417414
H38	3.463981	-1.24152	-0.22251
H39	6.158429	-1.2693	-0.02087
H40	6.923791	1.295667	0.46072
H41	4.6593	2.77306	0.546595
N42	1.969071	2.83887	-0.16136
C43	2.349544	3.178021	-1.47554
C44	1.835198	4.409179	-1.75816
C45	1.094456	4.854933	-0.61342
C46	1.169767	3.884406	0.341759
H47	1.98104	4.951991	-2.68163
H48	0.582525	5.801208	-0.50644
H49	-1.34695	-0.35444	-2.80909
H50	0.768051	3.841375	1.341301
H51	2.945815	2.501575	-2.06793

Table S238. $[Rh^{II}(PN)(TFA^{P})(TFAH^{N})]^{+}$

Atom	x	y	z
Rh1	0.524099	-0.29949	-0.20512
N2	-0.13669	-0.17142	1.773349
C3	0.558166	0.624141	2.66509
C4	0.177821	0.675691	4.037288
C5	-0.93706	-0.0938	4.455566
C6	-1.61206	-0.86562	3.539711
C7	-1.17852	-0.88449	2.200687
C8	0.930915	1.48602	4.926944

H9	-1.24351	-0.06532	5.497016
H10	-2.46902	-1.46703	3.820483
C11	1.665748	1.396314	2.21704
C12	2.380656	2.16972	3.117989
H13	-1.68151	-1.49069	1.456651
P14	2.041155	1.228136	0.457701
O15	-1.03158	-1.69654	-0.61844
C16	1.075408	-0.15987	-3.24082
O17	1.452629	-0.47205	-2.09326
O18	-0.08963	0.178878	-3.62869
C19	2.174582	-0.14698	-4.3306
F20	1.667992	0.061934	-5.53931
F21	3.042107	0.843591	-4.03929
F22	2.831078	-1.31015	-4.31226
C23	2.012335	2.213332	4.479534
H24	3.235846	2.745767	2.77876
H25	2.585021	2.82377	5.16974
H26	0.640678	1.518331	5.973163
C27	-3.27989	-2.14455	-1.2138
C28	-1.9838	-1.30969	-1.36433
O29	-1.98781	-0.33652	-2.14625
F30	-3.66746	-2.10653	0.084865
F31	-3.0462	-3.4203	-1.54466
F32	-4.26784	-1.66775	-1.96337
N33	3.664193	0.883141	0.192497
C34	4.171651	-0.41848	0.02481
C35	5.531528	-0.35682	0.105606
C36	5.897126	1.009823	0.338108
C37	4.753397	1.751611	0.397459
H38	3.509418	-1.24688	-0.17667
H39	6.206577	-1.19258	-0.01337
H40	6.901693	1.399931	0.427139
H41	4.595751	2.812268	0.516512
N42	1.896804	2.788446	-0.18564
C43	2.277245	3.122655	-1.49987
C44	1.680655	4.306672	-1.82453
C45	0.884993	4.723085	-0.70698
C46	1.012088	3.782846	0.273534
H47	1.810442	4.839734	-2.75619
H48	0.303337	5.631435	-0.63337
H49	-0.86454	0.024251	-2.91519
H50	0.591751	3.733292	1.265265

H51	2.943342	2.483791	-2.05895

Table S239. [$Rh^{III}(PN)(TFA)_2(CH_3^{ax}$-H-$TFA^P)]^{‡}$

Atom	x	y	z
Rh1	0.523319	-0.27587	0.164532
N2	-0.08832	-0.1452	2.168615
C3	0.735904	0.502134	3.059421
C4	0.426322	0.516057	4.449317
C5	-0.77663	-0.10377	4.874281
C6	-1.59449	-0.70258	3.948197
C7	-1.20799	-0.71123	2.591662
C8	1.326164	1.143274	5.348517
H9	-1.03528	-0.09425	5.929347
H10	-2.52577	-1.17882	4.233143
C11	1.911349	1.163706	2.59611
C12	2.771241	1.749947	3.509178
H13	-1.81108	-1.19067	1.828015
P14	2.121369	1.173058	0.791776
O15	-1.20883	-1.48793	-0.27175
C16	0.769296	-0.49877	-2.81292
O17	1.407476	-0.30341	-1.69511
O18	-0.34793	-0.92715	-3.02193
C19	1.688467	-0.10537	-4.00276
F20	1.088911	-0.30748	-5.17864
F21	2.028137	1.205812	-3.93046
F22	2.833327	-0.82	-3.98521
C23	2.482207	1.733971	4.891089
H24	3.679802	2.231873	3.164245
H25	3.171677	2.201955	5.586316
H26	1.087013	1.145041	6.408263
C27	-2.07916	-3.29474	-1.56996
C28	-0.91114	-2.5324	-0.91155
O29	0.233505	-3.04968	-0.98081
F30	-3.02662	-2.46417	-2.00598
F31	-2.62718	-4.10549	-0.63049
F32	-1.6619	-4.05544	-2.58415
N33	3.735391	0.848237	0.375981
C34	4.230429	-0.30453	-0.24869
C35	5.589096	-0.1938	-0.32679
C36	5.964069	1.059816	0.255021
C37	4.824088	1.686157	0.669779
H38	3.549684	-1.0407	-0.64071

H39	6.250056	-0.91677	-0.78371
H40	6.964092	1.464026	0.332281
H41	4.665722	2.667368	1.089827
N42	2.003194	2.796367	0.328699
C43	2.152514	3.204278	-1.00699
C44	1.942503	4.551303	-1.06027
C45	1.642446	5.004047	0.265772
C46	1.67106	3.922251	1.097582
H47	1.98553	5.155612	-1.95541
H48	1.419049	6.017882	0.567729
H49	0.978957	-2.33189	-0.13364
H50	1.451188	3.829219	2.14755
H51	2.362791	2.481919	-1.78142
O60	-0.61078	1.264233	-0.56798
C61	-1.16642	2.157952	0.182117
O62	-1.05473	2.344798	1.385781
C63	-2.08497	3.08251	-0.66542
F64	-2.59584	4.068272	0.087112
F65	-1.40139	3.643865	-1.67929
F66	-3.11029	2.382242	-1.18553
C59	1.714286	-2.17489	0.97264
H60	2.411642	-2.86656	0.482716
H61	2.356097	-1.49047	1.522969
H62	1.100138	-2.72575	1.688866

Table S240. $[Rh^{III}(PN)(TFA)_2(CH_3^{ax}\text{-}H\text{-}TFA^{N})]^{‡}$

Atom	x	y	z
Rh1	0.454246	-0.17252	-0.03136
N2	-0.1038	-0.2008	1.991588
C3	0.707288	0.404345	2.923586
C4	0.389753	0.338846	4.309843
C5	-0.81267	-0.30974	4.690692
C6	-1.61803	-0.86337	3.726531
C7	-1.22335	-0.79876	2.373445
C8	1.285117	0.915204	5.248141
H9	-1.07991	-0.35989	5.742565
H10	-2.54778	-1.36178	3.976542
C11	1.881818	1.090644	2.507978
C12	2.747395	1.612253	3.4535
H13	-1.81088	-1.24652	1.577294
P14	2.131808	1.164859	0.716801
O15	-1.29633	-1.2472	-0.42334

C16	1.79885	-0.77506	-2.50153
O17	0.947899	0.035655	-2.0457
O18	2.390965	-1.66942	-1.85392
C19	2.172585	-0.56112	-3.98247
F20	2.959587	-1.53825	-4.4378
F21	1.077298	-0.49247	-4.74443
F22	2.841166	0.609081	-4.08788
C23	2.447816	1.52414	4.830895
H24	3.66601	2.095846	3.133627
H25	3.136139	1.946662	5.555785
H26	1.039584	0.858132	6.304854
C27	-2.79466	-2.77648	-1.362
C28	-1.36163	-2.17845	-1.32004
O29	-0.49128	-2.61384	-2.05469
F30	-3.68674	-1.87023	-1.80095
F31	-3.1786	-3.15911	-0.11629
F32	-2.86145	-3.85077	-2.15556
N33	3.796812	0.863622	0.440425
C34	4.42681	-0.38516	0.443125
C35	5.779012	-0.18569	0.434061
C36	6.011312	1.225272	0.433528
C37	4.796025	1.851058	0.443438
H38	3.854199	-1.29566	0.423878
H39	6.527055	-0.96587	0.408183
H40	6.970644	1.723542	0.404874
H41	4.53462	2.897063	0.416238
N42	2.020015	2.784671	0.240499
C43	2.00123	3.164107	-1.10949
C44	2.059123	4.527251	-1.16484
C45	2.109745	5.019205	0.179076
C46	2.085558	3.944519	1.02276
H47	2.043892	5.11784	-2.06995
H48	2.133209	6.055417	0.487038
H49	1.802214	-1.72066	-0.6771
H50	2.0493	3.887697	2.097859
H51	1.928931	2.418676	-1.88721
O60	-0.7166	1.448294	-0.51379
C61	-1.11907	2.337144	0.330259
O62	-0.8229	2.489644	1.507712
C63	-2.10957	3.32128	-0.35398
F64	-2.54932	4.243038	0.515362
F65	-1.51097	3.96411	-1.37517

F66	-3.17964	2.665829	-0.84153
C59	1.410589	-2.20659	0.552
H60	0.430101	-2.62467	0.764454
H61	1.973754	-3.03099	0.090704
H62	1.935595	-1.94591	1.470696

Table S241. [$Rh^{III}(PN)(TFA^{ax})_2(CH_3{}^N$-H-$TFA^P$)]‡

Atom	x	y	z
Rh1	0.414245	-0.00091	-0.32511
N2	-0.24658	-0.05783	1.693643
C3	0.643695	0.313376	2.668576
C4	0.357579	0.084514	4.044012
C5	-0.90597	-0.46601	4.377229
C6	-1.79374	-0.77463	3.37633
C7	-1.41862	-0.57051	2.03108
C8	1.34794	0.397175	5.010522
H9	-1.15256	-0.64142	5.420413
H10	-2.77004	-1.19473	3.59036
C11	1.879482	0.913238	2.302806
C12	2.8344	1.174308	3.268991
H13	-2.06899	-0.85445	1.212375
P14	2.055315	1.287608	0.54261
O15	-1.2614	-1.27145	-0.74368
C23	2.568385	0.910295	4.630745
H24	3.799236	1.580022	2.979231
H25	3.329282	1.122168	5.375129
H26	1.130357	0.20947	6.058391
C27	-2.86244	-2.14321	-2.26355
C28	-1.56716	-1.35909	-1.96373
O29	-0.92304	-0.88543	-2.92449
F30	-3.85559	-1.70477	-1.4663
F31	-2.67033	-3.44939	-2.01354
F32	-3.24669	-2.00242	-3.53416
N33	3.700078	0.999491	0.188081
C34	4.356953	-0.23045	0.336482
C35	5.623081	-0.09366	-0.16082
C36	5.764961	1.246052	-0.64529
C37	4.582802	1.89702	-0.43375
H38	3.846211	-1.07862	0.762524
H39	6.374755	-0.87077	-0.17626
H40	6.64603	1.682426	-1.09534
H41	4.278675	2.908342	-0.6511

N42	1.95065	2.971088	0.371879
C43	1.539203	3.626059	-0.79861
C44	1.78865	4.960757	-0.64961
C45	2.375215	5.155815	0.641474
C46	2.469501	3.935289	1.246581
H47	1.552425	5.725714	-1.37597
H48	2.67307	6.097627	1.081657
H49	0.212641	-0.39835	-2.41654
H50	2.832634	3.659793	2.222713
H51	1.057165	3.078116	-1.59123
O53	1.538174	-1.62745	0.292006
C54	1.584637	-2.69644	-0.44682
O55	1.183672	-2.87765	-1.58068
C56	2.257524	-3.85576	0.337563
F57	2.426485	-4.93734	-0.42671
F58	3.475245	-3.48647	0.807708
F59	1.503979	-4.20454	1.401859
O60	-0.78639	1.540507	-0.9588
C61	-1.31622	2.393268	-0.13882
O62	-1.1412	2.532947	1.06077
C63	-2.28591	3.337052	-0.90086
F64	-2.80216	4.267379	-0.08887
F65	-1.6426	3.970791	-1.9051
F66	-3.30616	2.638853	-1.43896
C59	1.468984	0.087713	-2.37599
H60	1.491621	1.138903	-2.66093
H61	2.402535	-0.22841	-1.91569
H62	1.431898	-0.51677	-3.29348

Table S242. $[Rh^{III\text{-}I}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-\ddagger}$

Atom	x	y	z
Rh1	-0.55838	1.23821	2.321158
N2	1.222855	2.313704	2.327973
C3	2.363903	1.749264	1.796939
C4	3.589712	2.473308	1.73957
C5	3.605669	3.800524	2.236419
C6	2.454792	4.33342	2.763609
C7	1.278679	3.555831	2.795771
C8	4.736094	1.831099	1.206613
H9	4.528469	4.373507	2.20011
H10	2.424695	5.342278	3.160998
C11	2.308459	0.411236	1.329241

C12	3.455115	-0.18919	0.842708
H13	0.352707	3.946609	3.202449
P14	0.687701	-0.41877	1.560825
O15	-1.59754	3.018181	2.90602
C16	-2.68168	-0.83577	2.360175
O17	-2.44882	0.415324	2.258721
O18	-1.89159	-1.77726	2.453376
C19	-4.19079	-1.19314	2.370579
F20	-4.52823	-1.74598	3.556227
F21	-5.00129	-0.14154	2.16733
F22	-4.4585	-2.10438	1.408071
C23	4.670914	0.526131	0.7711
H24	3.420574	-1.22606	0.522232
H25	5.556871	0.037013	0.376695
H26	5.670098	2.385341	1.160254
C27	-2.97204	4.908034	2.954688
C28	-2.29384	3.763114	2.155548
O29	-2.46939	3.751818	0.929058
F30	-2.01554	5.736108	3.451783
F31	-3.67971	4.436958	3.997046
F32	-3.79489	5.652044	2.200293
N33	1.177085	-1.9016	2.298572
C34	1.501755	-2.01792	3.648884
C35	2.093203	-3.23882	3.844249
C36	2.144166	-3.90408	2.582914
C37	1.591232	-3.06687	1.648304
H38	1.323797	-1.22577	4.361517
H39	2.443193	-3.61151	4.79702
H40	2.525652	-4.89724	2.383904
H41	1.411802	-3.20412	0.594785
N42	0.331358	-0.99535	-0.03189
C43	-0.6689	-1.9145	-0.35344
C44	-0.76149	-1.98545	-1.71931
C45	0.184548	-1.06785	-2.26881
C46	0.83538	-0.46801	-1.22276
H47	-1.4413	-2.62449	-2.26666
H48	0.359979	-0.85623	-3.31424
H49	1.586721	0.303122	-1.21613
H50	-1.21962	-2.40859	0.432095
O51	0.581382	2.973342	-0.73725
C52	-0.33807	2.778977	-1.50691
O53	-1.62347	2.779897	-1.27053

C54	-0.05276	2.554016	-3.01254
F55	-0.08674	3.743927	-3.65627
F56	1.174909	2.032437	-3.19457
F57	-0.94148	1.743108	-3.60443
H58	-1.85018	3.053247	-0.31264
O59	-0.42885	0.525024	6.669326
C60	-0.45163	0.798309	4.645542
H61	-0.84217	-0.20152	4.53682
H62	0.613575	0.94623	4.702
H63	-1.13153	1.620822	4.808974
C64	0.706023	0.087152	7.045348
O65	1.713889	-0.19633	6.390047
C66	0.77072	-0.10064	8.592027
F67	-0.12128	-1.02791	9.009686
F68	1.987525	-0.50148	9.008799
F69	0.485733	1.051778	9.241955

Table S243. $[Rh^{III\text{-}I}(PN)(TFA^{N})(TFAH^{ax})(TFAH^{P})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Atom	x	y	z
Rh1	1.272928	0.469537	0.659586
N2	0.287312	-1.36683	0.73277
C3	-0.32252	-1.75296	1.909271
C4	-0.92813	-3.03444	2.036251
C5	-0.87089	-3.91466	0.923027
C6	-0.22958	-3.51345	-0.21947
C7	0.346067	-2.22568	-0.27852
C8	-1.53041	-3.38416	3.270482
H9	-1.31763	-4.90179	1.000275
H10	-0.1264	-4.16488	-1.07884
C11	-0.32382	-0.86389	3.01777
C12	-0.90796	-1.24771	4.213947
H13	0.865632	-1.89605	-1.16726
P14	0.539134	0.696375	2.702398
O15	1.704486	0.132661	-1.53475
C16	2.12878	3.33002	0.178758
O17	2.383811	2.266475	0.793706
O18	1.331452	3.513811	-0.7812
C19	2.867734	4.581984	0.719455
F20	2.123855	5.121204	1.715677
F21	4.069136	4.27164	1.218739
F22	3.023683	5.508169	-0.23158
C23	-1.51982	-2.51183	4.338229

H24	-0.88634	-0.57742	5.067106
H25	-1.97478	-2.7964	5.281586
H26	-1.99105	-4.36368	3.364653
C27	1.783755	-0.11247	-3.90343
C28	1.606533	0.716376	-2.61011
O29	1.403733	1.975718	-2.8255
F30	1.20748	-1.31435	-3.74632
F31	3.092687	-0.2884	-4.13218
F32	1.234761	0.490517	-4.96149
N33	1.556434	1.069707	4.014967
C34	2.940715	0.858913	4.048652
C35	3.376556	1.080394	5.323859
C36	2.240539	1.433614	6.119678
C37	1.140115	1.418948	5.310053
H38	3.476008	0.592946	3.153569
H39	4.403573	1.014385	5.654281
H40	2.241597	1.690011	7.170322
H41	0.109744	1.668458	5.507407
N42	-0.66909	1.891637	2.960143
C43	-0.3958	3.262649	3.046558
C44	-1.57853	3.942349	2.945029
C45	-2.62061	2.97921	2.766148
C46	-2.04435	1.737235	2.761507
H47	-1.69268	5.015952	3.000852
H48	-3.6769	3.180506	2.658215
H49	-2.48004	0.758603	2.641923
H50	0.614672	3.616427	3.17957
O51	-1.08922	1.282737	-0.51448
C52	-1.77791	2.281627	-0.59621
O53	-1.3696	3.528054	-0.67207
C54	-3.31638	2.169328	-0.69017
F55	-3.94008	3.23957	-0.18158
F56	-3.66751	2.048282	-1.98407
F57	-3.73852	1.077703	-0.03567
C58	3.084825	-0.76989	0.983673
H59	3.876283	-0.0305	1.030729
H60	2.882883	-1.33181	1.883294
H61	2.89815	-1.26769	0.044284
H62	-0.37526	3.556805	-0.65735
H63	1.353656	2.518576	-1.96203
O64	4.660812	-2.29799	0.838178
C65	4.189432	-3.23321	0.129636

O66	3.081231	-3.34385	-0.42808
C67	5.155278	-4.43643	-0.09563
F68	5.455702	-4.55786	-1.40846
F69	6.314927	-4.32751	0.576122
F70	4.57015	-5.59321	0.291875

Table S244. $[Rh^{III\text{-}I}(PN)(TFA^{P})(TFAH^{ax})(TFAH^{N})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Atom	x	y	z
Rh1	-0.68514	0.465395	2.07808
N2	0.315355	-0.77376	0.762096
C3	-0.24177	-1.98468	0.408628
C4	0.485027	-2.92275	-0.37762
C5	1.787648	-2.57011	-0.80697
C6	2.310292	-1.35048	-0.44827
C7	1.545542	-0.47859	0.349535
C8	-0.11664	-4.17267	-0.67451
H9	2.361672	-3.2731	-1.40369
H10	3.30696	-1.04694	-0.74791
C11	-1.54918	-2.30723	0.859593
C12	-2.09565	-3.54345	0.565061
H13	1.938212	0.474506	0.682989
P14	-2.3118	-1.03537	1.899327
O15	1.005049	1.823299	2.132814
C16	-2.40184	2.669599	3.418674
O17	-1.65126	1.695722	3.528386
O18	-2.83044	3.250885	2.35115
C19	-3.00363	3.262247	4.712292
F20	-3.24174	4.569556	4.587752
F21	-4.17109	2.629516	4.948641
F22	-2.18777	3.059471	5.746413
C23	-1.37574	-4.47945	-0.20892
H24	-3.07943	-3.80223	0.944911
H25	-1.81851	-5.44595	-0.42657
H26	0.443994	-4.89248	-1.26399
C27	2.122758	3.725324	2.996616
C28	1.010106	3.085604	2.127225
O29	0.271599	3.867871	1.486558
F30	3.284742	3.695857	2.309644
F31	2.294674	3.043629	4.139127
F32	1.843163	4.998108	3.300262
N33	-3.07582	-1.81281	3.213435
C34	-2.46846	-2.17075	4.427356

C35	-3.32141	-2.99064	5.108452
C36	-4.4921	-3.17133	4.307016
C37	-4.32522	-2.46123	3.152688
H38	-1.47718	-1.84059	4.682433
H39	-3.1274	-3.41945	6.081445
H40	-5.36929	-3.75025	4.562242
H41	-4.98414	-2.30883	2.313816
N42	-3.71013	-0.54515	1.035578
C43	-4.68269	0.316281	1.554618
C44	-5.54509	0.646526	0.544834
C45	-5.09168	-0.00459	-0.64337
C46	-3.96699	-0.71599	-0.32624
H47	-6.41613	1.279225	0.644897
H48	-5.54631	0.044648	-1.62286
H49	-3.31764	-1.31892	-0.93929
H50	-4.68938	0.575345	2.602843
O51	-2.34842	2.248531	0.049193
C52	-1.50461	2.425505	-0.83175
O53	-0.39773	3.075742	-0.75604
C54	-1.732	1.739933	-2.19972
F55	-1.3998	0.431759	-2.07622
F56	-3.01607	1.81472	-2.56107
F57	-0.97881	2.270795	-3.16631
C58	0.427638	-0.61797	3.676693
H59	-0.1384	-0.28378	4.537041
H60	0.314437	-1.62531	3.299902
H61	1.38731	-0.13367	3.540857
H62	-0.18765	3.416293	0.232979
H63	-2.5188	2.838333	1.470771
O64	1.442642	-1.95094	5.162511
C65	1.44999	-3.10389	4.635396
O66	0.994727	-3.48966	3.54479
C67	2.084234	-4.20124	5.544079
F68	2.595519	-5.21732	4.8218
F69	3.070578	-3.72438	6.326155
F70	1.135475	-4.72345	6.360015

Table S245. [$Rh^{III\text{-}I}$(PN)(TFA^{ax})$_2$($TFAH^{P}$)(CH_3^N-TFA)]$^{-‡}$

Atom	x	y	z
Rh1	0.477139	-0.16178	-0.58794
N2	-0.23627	0.611406	2.294086
C3	0.94491	0.381787	2.926307

C4	1.019955	-0.09998	4.266423
C5	-0.20941	-0.3315	4.936749
C6	-1.39387	-0.10114	4.277046
C7	-1.35871	0.368435	2.938126
C8	2.296554	-0.32953	4.841727
H9	-0.19794	-0.69855	5.960683
H10	-2.35038	-0.28018	4.758767
C11	2.143065	0.625619	2.19114
C12	3.367891	0.373123	2.777505
H13	-2.27198	0.542177	2.372814
P14	1.921582	1.14813	0.449088
O15	-1.17153	-1.40598	-1.41746
C23	3.440609	-0.10154	4.110562
H24	4.282723	0.534528	2.215904
H25	4.414919	-0.29318	4.551089
H26	2.356667	-0.70028	5.862572
C27	-3.54282	-1.72455	-1.36641
C28	-2.13948	-1.72226	-0.72335
O29	-2.13954	-2.16363	0.489519
F30	-3.62955	-0.82143	-2.346
F31	-4.50941	-1.48877	-0.47135
F32	-3.76574	-2.94821	-1.90533
N33	3.55574	1.246597	-0.11401
C34	4.240236	0.209436	-0.75107
C35	5.548976	0.5862	-0.89706
C36	5.691762	1.890944	-0.33159
C37	4.465783	2.275119	0.146149
H38	3.74186	-0.69654	-1.05585
H39	6.310485	-0.0068	-1.38376
H40	6.591607	2.491549	-0.29962
H41	4.141127	3.189139	0.618113
N42	1.551803	2.821663	0.644188
C43	1.044179	3.642649	-0.36048
C44	0.994425	4.926205	0.115584
C45	1.48715	4.910463	1.456934
C46	1.824683	3.617414	1.758432
H47	0.622437	5.781849	-0.43113
H48	1.571091	5.753774	2.129787
H49	-1.16965	-2.30672	0.852977
H50	2.221784	3.182322	2.661206
H51	0.716208	3.218249	-1.29502
O53	1.64413	-1.79714	0.06957

C54	1.225311	-2.63975	0.911121
O55	0.091907	-2.78343	1.413989
C56	2.307519	-3.61263	1.444201
F57	1.820338	-4.86217	1.564678
F58	3.393793	-3.66519	0.663097
F59	2.702586	-3.20783	2.675375
O60	-0.65004	1.396244	-1.35133
C61	-1.85018	1.557915	-0.93241
O62	-2.50151	0.918014	-0.10665
C63	-2.58252	2.730364	-1.63904
F64	-3.31436	3.441198	-0.75778
F65	-1.75114	3.592661	-2.25897
F66	-3.4321	2.245277	-2.57273
C59	1.519091	-0.45152	-2.712
H60	0.548623	-0.46215	-3.18478
H61	2.074355	0.470883	-2.67251
H62	1.961353	-1.35831	-2.33301
O63	2.351743	-0.82334	-4.49416
C64	3.452435	-1.45515	-4.35975
O65	4.032551	-1.85641	-3.34929
C66	4.135873	-1.79481	-5.71965
F67	3.648657	-1.0956	-6.76424
F68	5.465878	-1.56106	-5.6694
F69	3.973677	-3.10946	-6.00952

Table S246. [$Rh^{III\text{-}I}$(PN)(TFA^{ax})($TFAH^{ax}$)($TFAH^{P}$)($CH_3{}^{N}$-TFA)]‡

Atom	x	y	z
Rh1	0.282101	-0.07897	-0.39608
N2	-0.39513	0.829319	2.478326
C3	0.840853	0.530606	2.993887
C4	0.962161	-0.04145	4.298822
C5	-0.22238	-0.32665	5.021022
C6	-1.44804	-0.05443	4.460325
C7	-1.48037	0.535868	3.182899
C8	2.249517	-0.32551	4.826053
H9	-0.14445	-0.76777	6.011164
H10	-2.37531	-0.2701	4.979349
C11	2.028748	0.76613	2.229865
C12	3.261455	0.457052	2.777748
H13	-2.43121	0.791692	2.720824
P14	1.904545	1.187643	0.457772
O15	-1.62959	-1.07991	-0.81125

C16	3.376246	-0.07106	4.084064
H17	4.161336	0.602576	2.189122
H18	4.360608	-0.29755	4.481042
H19	2.323158	-0.76002	5.819231
C20	-3.54285	-2.11941	-1.78196
C21	-2.03611	-2.0657	-1.43891
O22	-1.37956	-3.09598	-1.81834
F23	-4.02069	-0.88458	-1.98634
F24	-4.20173	-2.66175	-0.73884
F25	-3.7782	-2.85815	-2.8678
N26	3.494388	1.161423	-0.13898
C27	4.136704	0.071315	-0.7501
C28	5.458947	0.384676	-0.88355
C29	5.664592	1.692391	-0.33742
C30	4.461864	2.152758	0.117466
H31	3.605223	-0.81202	-1.06963
H32	6.196885	-0.25051	-1.35281
H33	6.595648	2.242353	-0.30643
H34	4.180895	3.091402	0.568586
N35	1.590412	2.874797	0.468059
C36	1.411112	3.638396	-0.68818
C37	1.228711	4.943482	-0.31792
C38	1.302447	5.003922	1.108589
C39	1.529384	3.735414	1.56869
H40	1.061909	5.770621	-0.99367
H41	1.197078	5.885562	1.725565
H42	-0.40478	-3.15356	-1.3939
H43	1.651573	3.357361	2.570794
H44	1.447327	3.176897	-1.66341
O45	1.353401	-1.63098	0.460031
C46	1.447854	-2.84572	0.092174
O47	0.785834	-3.48647	-0.73663
C48	2.555621	-3.60333	0.868076
F49	2.776724	-4.8175	0.368489
F50	3.706943	-2.91064	0.852478
F51	2.174226	-3.73906	2.160582
O52	-0.80549	1.521412	-1.22008
C53	-1.48612	2.303002	-0.54922
O54	-1.56408	2.394468	0.736872
C55	-2.39982	3.312398	-1.27609
F56	-2.10783	4.561056	-0.88726
F57	-2.2509	3.220399	-2.5963

F58	-3.67874	3.051734	-0.9593
C59	1.169479	-0.41545	-2.41914
H60	0.2522	-0.49402	-2.99164
H61	1.750536	0.482134	-2.57268
H62	1.692824	-1.31439	-2.12668
O63	2.222022	-0.99694	-4.26897
C64	3.142425	-1.79055	-3.91176
O65	3.41523	-2.2514	-2.78884
C66	4.082475	-2.26106	-5.06333
F67	3.81003	-1.683	-6.2465
F68	5.369633	-1.97662	-4.76086
F69	3.992379	-3.59771	-5.23237
H70	-0.94703	1.750919	1.272062

Table S247. $[Rh^{III\text{-}II}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{\ddagger}$

Atom	x	y	z
Rh1	-0.21663	1.451914	1.965722
N2	1.565196	2.563988	1.863528
C3	2.761054	1.888005	1.767447
C4	4.001643	2.576396	1.904162
C5	3.969529	3.982676	2.080072
C6	2.758996	4.631256	2.128914
C7	1.568917	3.880991	2.032106
C8	5.204684	1.826113	1.873417
H9	4.903283	4.52864	2.181827
H10	2.692658	5.704886	2.265046
C11	2.746424	0.484415	1.543985
C12	3.94264	-0.21116	1.533457
H13	0.595746	4.347297	2.134897
P14	1.088957	-0.23852	1.240415
O15	-1.15436	3.208357	2.749431
C16	-2.35158	-0.57645	1.749766
O17	-1.9666	0.466262	2.401545
O18	-1.7813	-1.15314	0.832128
C19	-3.69193	-1.1256	2.300668
F20	-4.1725	-2.10977	1.533089
F21	-3.49283	-1.62211	3.543262
F22	-4.62283	-0.16037	2.383982
C23	5.173509	0.459081	1.711036
H24	3.940074	-1.28625	1.388222
H25	6.096651	-0.11166	1.705496
H26	6.149617	2.349062	1.991047

C27	-2.7284	4.77009	3.509913
C28	-2.34449	3.609164	2.556974
O29	-3.1942	3.232202	1.737844
F30	-1.84398	5.784137	3.364531
F31	-2.67454	4.35785	4.790526
F32	-3.95139	5.245822	3.268573
N33	1.078099	-1.78282	1.955842
C34	0.457599	-2.10703	3.165848
C35	0.810576	-3.38389	3.502778
C36	1.675038	-3.88054	2.477417
C37	1.826942	-2.894	1.542938
H38	-0.21077	-1.41131	3.644224
H39	0.468235	-3.9186	4.377559
H40	2.116045	-4.86651	2.424591
H41	2.346074	-2.88551	0.597645
N42	1.220064	-0.651	-0.41421
C43	0.411069	-1.56133	-1.10867
C44	0.787268	-1.54776	-2.4219
C45	1.841473	-0.59153	-2.57016
C46	2.085037	-0.04797	-1.34217
H47	0.350434	-2.15655	-3.2013
H48	2.360205	-0.33294	-3.48303
H49	2.792551	0.704321	-1.03684
H50	-0.36171	-2.10415	-0.59214
O51	-0.67997	1.963652	-0.26567
C52	-1.76774	1.804999	-0.82823
O53	-2.9491	1.895236	-0.32696
C54	-1.7969	1.460087	-2.33757
F55	-2.62596	2.296301	-2.98517
F56	-0.5792	1.570287	-2.87668
F57	-2.23658	0.204838	-2.51113
C58	0.166482	1.205477	4.487618
H59	-0.7646	0.654877	4.46434
H60	1.070564	0.734898	4.119726
H61	0.081886	2.283105	4.454276
H62	-2.97413	2.343542	0.625724
O63	0.5248	1.022266	6.167129
V64	1.936623	1.030068	7.031197
Cl65	2.203219	2.951542	7.993453
Cl66	1.988327	-0.67377	8.361464
Cl67	3.452036	0.774773	5.481187

Table S248. $[Rh^{I-III}(PN)(H^N)(CH_3{}^N)(TFA^P)]^{\ddagger}$

Atom	x	y	z
Rh1	0.543012	-0.2951	-0.22348
N2	-0.07055	-0.2084	1.879003
C3	0.594818	0.653102	2.719906
C4	0.232547	0.764631	4.093863
C5	-0.83637	-0.04174	4.564582
C6	-1.48325	-0.88857	3.697169
C7	-1.06856	-0.94435	2.347632
C8	0.944828	1.670844	4.920328
H9	-1.13155	0.024213	5.608221
H10	-2.30666	-1.5146	4.023082
C11	1.654246	1.45062	2.199318
C12	2.323039	2.322496	3.040215
H13	-1.55424	-1.58787	1.61851
P14	2.038002	1.168866	0.428162
O15	-0.9927	-1.68309	-0.48317
C23	1.968629	2.433413	4.403716
H24	3.131324	2.933312	2.651713
H25	2.509146	3.12627	5.041154
H26	0.666802	1.754081	5.967581
C27	-2.95745	-2.72746	-1.20601
C28	-1.90125	-1.60531	-1.39861
O29	-2.02298	-0.81589	-2.32089
F30	-3.46512	-2.69597	0.055532
F31	-2.4086	-3.94829	-1.38471
F32	-3.9852	-2.60931	-2.05533
N33	3.715116	0.77627	0.369624
C34	4.166703	-0.54153	0.27176
C35	5.518617	-0.55355	0.484115
C36	5.92786	0.794642	0.729238
C37	4.813361	1.587897	0.66417
H38	3.470452	-1.33495	0.046832
H39	6.15368	-1.42788	0.451661
H40	6.935733	1.141558	0.913223
H41	4.69959	2.656633	0.75292
N42	2.135418	2.780133	-0.186
C43	2.760165	3.122099	-1.38765
C44	2.305567	4.354216	-1.77657
C45	1.346064	4.786223	-0.8101
C46	1.245003	3.805274	0.13997
H47	2.635707	4.898725	-2.65047

H48	0.80367	5.7216	-0.80806
H50	0.62953	3.741112	1.023285
H51	3.486221	2.461703	-1.83572
C47	1.306987	-0.75959	-2.15589
H45	0.526716	-0.92981	-2.8976
H46	2.081883	-0.1064	-2.55875
H49	1.743738	-1.71937	-1.85646
H52	0.320033	0.471026	-1.53723

Table S249. $[Rh^{I\text{-}III}(PN)(H^{N}\text{-}TFA)(CH_3{}^{N})(TFA^{P})]^{\ddagger}$

Atom	x	y	z
Rh1	0.349466	0.01158	-0.27699
N2	0.008395	-0.15117	1.8007
C3	0.638428	0.736947	2.653447
C4	0.297677	0.815792	4.033922
C5	-0.68784	-0.07524	4.530095
C6	-1.28293	-0.9618	3.664211
C7	-0.9156	-0.96638	2.302212
C8	0.94098	1.791517	4.839583
H9	-0.96208	-0.03859	5.581405
H10	-2.04389	-1.65829	4.001319
C11	1.630907	1.60215	2.11632
C12	2.220836	2.550433	2.928683
H13	-1.39002	-1.6285	1.585894
P14	1.973273	1.271814	0.343544
O15	-1.1472	-1.50526	-0.58401
C23	1.871653	2.647742	4.295645
H24	2.948323	3.239286	2.510208
H25	2.344806	3.404215	4.915916
H26	0.672144	1.859773	5.89103
C27	-1.92533	-3.69157	-0.87217
C28	-0.75128	-2.67203	-0.93263
O29	0.360608	-3.08895	-1.24599
F30	-2.35206	-3.83871	0.415808
F31	-1.57731	-4.91661	-1.30817
F32	-2.99374	-3.29655	-1.59708
N33	3.53279	0.479195	0.42448
C34	3.724453	-0.83002	-0.00799
C35	5.005098	-1.20815	0.307476
C36	5.628991	-0.10401	0.967248
C37	4.707308	0.910143	1.033534
H38	2.908452	-1.36487	-0.47418

H39	5.447229	-2.17118	0.090745
H40	6.641932	-0.05933	1.346964
H41	4.785891	1.905778	1.440432
N42	2.536538	2.824632	-0.22615
C43	3.655384	3.087756	-1.01487
C44	3.608015	4.402185	-1.40599
C45	2.414141	4.968856	-0.86571
C46	1.768119	3.983883	-0.16129
H47	4.351196	4.902097	-2.01342
H48	2.060651	5.983756	-0.99029
H50	0.800842	3.967531	0.320183
H51	4.384727	2.318742	-1.21031
C47	0.596055	0.172264	-2.46731
H45	-0.2546	-0.06319	-3.11387
H46	1.213697	0.942683	-2.93726
H49	1.183237	-0.74824	-2.37577
H52	-0.24413	1.105523	-1.75446
O53	-1.17386	2.060364	-1.96687
C54	-1.60782	2.818521	-1.03685
O55	-1.2034	3.022461	0.108698
C56	-2.86993	3.603872	-1.50731
F57	-3.35979	4.414917	-0.54752
F58	-2.59164	4.383988	-2.57996
F59	-3.86896	2.767506	-1.87082

Table S250. $Rh^{I}(PN)(CH_3{}^{N})(TFAH^{P})$

Atom	x	y	z
Rh1	0.723757	-0.65183	-0.05523
N2	0.04069	-0.45426	2.029483
C3	0.621968	0.54065	2.789202
C4	0.253501	0.744241	4.152309
C5	-0.73166	-0.1088	4.713345
C6	-1.29257	-1.09332	3.935571
C7	-0.87456	-1.23102	2.594193
C8	0.881021	1.782845	4.887689
H9	-1.02814	0.027678	5.749871
H10	-2.04791	-1.76593	4.327959
C11	1.609547	1.377306	2.190608
C12	2.197407	2.376125	2.945777
H13	-1.3029	-1.99821	1.95573
P14	2.028875	0.955334	0.448178
O15	-1.06188	-2	-0.54692

C23	1.833009	2.581595	4.296185
H24	2.951652	3.015169	2.498696
H25	2.310719	3.374574	4.863725
H26	0.596749	1.934769	5.925749
C27	-3.19654	-2.00386	-1.63437
C28	-1.88756	-1.33798	-1.17159
O29	-1.77371	-0.07872	-1.48441
F30	-3.8507	-2.47381	-0.55704
F31	-2.9128	-3.03426	-2.44369
F32	-3.99802	-1.15434	-2.28282
N33	3.749259	0.73934	0.450568
C34	4.327554	-0.52873	0.471803
C35	5.672867	-0.39061	0.691307
C36	5.945214	1.006999	0.816665
C37	4.757711	1.676755	0.674376
H38	3.709822	-1.40013	0.314909
H39	6.390468	-1.198	0.7397
H40	6.91145	1.467454	0.974334
H41	4.540203	2.732978	0.664929
N42	2.008786	2.527456	-0.30079
C43	2.628265	2.827031	-1.51233
C44	2.111867	4.005822	-1.98635
C45	1.118837	4.443698	-1.05856
C46	1.062353	3.518354	-0.04802
H47	2.422249	4.509845	-2.89138
H48	0.527191	5.347052	-1.11843
H50	0.446154	3.479996	0.836439
H51	3.389882	2.176654	-1.91342
C47	1.422839	-0.87444	-2.00108
H45	0.819606	-1.65069	-2.49273
H46	1.37725	0.033755	-2.61513
H49	2.466336	-1.2158	-1.99437
H52	-0.85145	0.212243	-1.11276

Table S251. $Rh^{III}(PN)(H^{ax})(CH_3{}^{N})(\kappa^2\text{-}TFA^{ax,P})$

Atom	x	y	z
Rh1	1.065596	-0.48378	-0.00055
N2	0.402461	-0.35966	2.156791
C3	0.839392	0.725888	2.873986
C4	0.43886	0.926322	4.227998
C5	-0.41788	-0.04087	4.814775
C6	-0.83128	-1.12103	4.073471

C7	-0.396	-1.24175	2.733856
C8	0.907595	2.069823	4.923264
H9	-0.7349	0.08601	5.846215
H10	-1.48362	-1.88027	4.491053
C11	1.708638	1.669668	2.248689
C12	2.142887	2.771564	2.964505
H13	-0.7063	-2.0778	2.113236
P14	2.235221	1.258954	0.542137
O15	2.115381	-2.57701	0.403625
C16	1.739365	2.974992	4.303379
H17	2.800569	3.49539	2.494197
H18	2.092883	3.849719	4.840447
H19	0.598069	2.219527	5.953976
C20	0.795853	-4.59553	0.276485
C21	1.003238	-3.07661	0.117714
O22	-0.01404	-2.40754	-0.23476
F23	0.040852	-4.82136	1.380978
F24	1.953382	-5.25199	0.427582
F25	0.148132	-5.11728	-0.77769
N26	3.936357	1.060243	0.601528
C27	4.547779	-0.19884	0.651238
C28	5.87499	-0.01542	0.927264
C29	6.103707	1.390345	1.063618
C30	4.908979	2.028966	0.872361
H31	3.968419	-1.09568	0.484979
H32	6.611819	-0.80196	1.011534
H33	7.049281	1.876324	1.263219
H34	4.661518	3.078416	0.858086
N35	2.158123	2.782935	-0.25269
C36	2.837543	3.086609	-1.43634
C37	2.247866	4.184511	-2.00281
C38	1.148485	4.563214	-1.17183
C39	1.101209	3.686481	-0.12148
H40	2.574854	4.675474	-2.90889
H41	0.478352	5.398062	-1.32369
H42	0.421681	3.62294	0.713697
H43	3.685851	2.497075	-1.74677
C44	1.647893	-0.56256	-1.98249
H45	0.899895	-1.18227	-2.48558
H46	1.707481	0.410544	-2.47502
H47	2.623771	-1.05912	-2.01975
H48	0.043113	0.569097	-0.45356

Table S252. $Rh^{III}(PN)(H^{ax})(CH_3{}^N)(TFA^P)$

Atom	x	y	z
Rh1	0.549008	-0.27263	-0.28772
N2	-0.05506	-0.24158	1.889044
C3	0.558788	0.677646	2.702538
C4	0.1814	0.816313	4.071089
C5	-0.84325	-0.03346	4.56467
C6	-1.4354	-0.94468	3.723948
C7	-1.01049	-1.01616	2.377328
C8	0.832477	1.790122	4.870055
H9	-1.1486	0.051598	5.604233
H10	-2.22371	-1.6057	4.067556
C11	1.581969	1.514749	2.162402
C12	2.186414	2.455675	2.977966
H13	-1.4589	-1.71002	1.670657
P14	2.027633	1.202755	0.410126
O15	-0.87508	-1.74385	-0.58452
C16	1.812391	2.594893	4.333291
H17	2.954961	3.10614	2.573599
H18	2.303397	3.342656	4.948271
H19	0.541433	1.893297	5.91204
C20	-2.85623	-2.86229	-1.12649
C21	-1.9781	-1.58738	-1.24153
O22	-2.39465	-0.62074	-1.85633
F23	-3.17847	-3.0851	0.178271
F24	-2.20901	-3.95861	-1.5707
F25	-4.00215	-2.75364	-1.80934
N26	3.684972	0.741354	0.413604
C27	4.094839	-0.58011	0.218335
C28	5.434941	-0.66198	0.481316
C29	5.879767	0.64429	0.857658
C30	4.797639	1.481951	0.817533
H31	3.389473	-1.32687	-0.11401
H32	6.040146	-1.55374	0.396921
H33	6.890264	0.935104	1.110847
H34	4.718174	2.542341	0.996666
N35	2.188865	2.799359	-0.21504
C36	2.906475	3.116712	-1.37207
C37	2.484774	4.340047	-1.81965
C38	1.451491	4.79042	-0.94158
C39	1.274679	3.830085	0.018153
H40	2.882185	4.866554	-2.6763

H41	0.910726	5.724763	-1.00213
H42	0.59214	3.784375	0.852101
H43	3.661679	2.445197	-1.74947
C44	1.107232	-0.35002	-2.27144
H45	0.205729	-0.52344	-2.86153
H46	1.622248	0.538839	-2.6438
H47	1.775266	-1.21976	-2.35299
H48	-0.26791	0.918075	-0.73393

Table S253. $Rh^{III}(PN)(H^{ax})(CH_3{}^{N})(TFA^{P})(TFAH^{ax})$

Atom	x	y	z
Rh1	0.631066	-0.27286	-0.20709
N2	-0.13266	0.010891	1.900916
C3	0.661124	0.733545	2.752757
C4	0.348891	0.842176	4.140171
C5	-0.82853	0.199888	4.605001
C6	-1.61861	-0.49273	3.719179
C7	-1.22796	-0.56695	2.362132
C8	1.220794	1.574792	4.985743
H9	-1.09038	0.265467	5.657901
H10	-2.52802	-0.99044	4.038822
C11	1.819673	1.386323	2.236922
C12	2.647646	2.084691	3.097092
H13	-1.81718	-1.11003	1.627869
P14	2.124167	1.187403	0.442377
O15	-1.20521	-1.34298	-0.5909
C16	2.350222	2.175813	4.475794
H17	3.544152	2.561737	2.713475
H18	3.018408	2.726692	5.130455
H19	0.984538	1.648777	6.044173
C20	-2.98464	-2.52562	-1.56481
C21	-1.47092	-2.36779	-1.27025
O22	-0.71353	-3.25558	-1.71813
F23	-3.42933	-1.49294	-2.30502
F24	-3.67525	-2.52874	-0.40088
F25	-3.26713	-3.6597	-2.2152
N26	3.81255	0.950528	0.264252
C27	4.415463	-0.30934	0.236959
C28	5.770985	-0.13953	0.308801
C29	6.029389	1.26442	0.389783
C30	4.824484	1.913819	0.372486
H31	3.81322	-1.20022	0.189302

H32	6.50326	-0.93482	0.294317
H33	6.998199	1.743335	0.436089
H34	4.583656	2.964638	0.377666
N35	2.027438	2.806904	-0.13709
C36	2.396825	3.184893	-1.43008
C37	1.831823	4.40189	-1.70256
C38	1.062202	4.786722	-0.56093
C39	1.181953	3.793692	0.373829
H40	1.965325	4.966911	-2.61482
H41	0.499213	5.701596	-0.43692
H42	0.759064	3.700933	1.361242
H43	3.040087	2.553308	-2.02321
C44	1.375443	-0.51027	-2.13075
H45	0.686606	-1.17172	-2.66231
H46	1.459854	0.431067	-2.67906
H47	2.363011	-0.98201	-2.07588
H48	-0.07898	0.946005	-0.78244
O49	1.715577	-2.19524	0.634524
C50	1.920495	-3.35195	0.263573
O51	1.362586	-4.01786	-0.68103
C52	3.033017	-4.14005	0.997301
F53	2.985958	-5.45272	0.754778
F54	4.236845	-3.67745	0.590493
F55	2.940316	-3.94655	2.322324
H56	0.51543	-3.54616	-1.14521

Table S254. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{ax})$

Atom	x	y	z
Rh1	0.89341	-0.26136	-0.21815
N2	-0.02863	-0.05154	1.851854
C3	0.644017	0.799564	2.689719
C4	0.273557	0.931751	4.059919
C5	-0.81797	0.158527	4.530926
C6	-1.47556	-0.68403	3.66811
C7	-1.03795	-0.75877	2.327035
C8	1.011579	1.807697	4.896519
H9	-1.11524	0.238023	5.573097
H10	-2.30931	-1.29622	3.993982
C11	1.742958	1.558029	2.187488
C12	2.443062	2.393665	3.038071
H13	-1.52901	-1.42986	1.626929
P14	2.17979	1.305062	0.43424

O15	1.763513	-2.1543	0.335262
C16	2.076964	2.520226	4.397035
H17	3.294238	2.954671	2.667182
H18	2.645693	3.181719	5.042911
H19	0.726006	1.89822	5.941086
C20	2.477676	-3.89159	1.754559
C21	2.219016	-2.38064	1.515117
O22	2.486773	-1.58459	2.410807
F23	3.433881	-4.34983	0.917598
F24	1.357404	-4.61666	1.532428
F25	2.879808	-4.14309	3.010651
N26	3.853105	1.034319	0.282388
C27	4.445065	-0.21669	0.071782
C28	5.799161	-0.06857	0.1738
C29	6.071095	1.306486	0.46532
C30	4.875896	1.964916	0.53216
H31	3.828244	-1.07764	-0.13256
H32	6.525758	-0.85875	0.046801
H33	7.044051	1.761722	0.592337
H34	4.649222	3.009091	0.675857
N35	2.117856	2.897179	-0.2077
C36	2.640011	3.253613	-1.45449
C37	2.153972	4.488296	-1.78865
C38	1.282033	4.910694	-0.73648
C39	1.259674	3.920201	0.206944
H40	2.403942	5.04	-2.68428
H41	0.742182	5.845696	-0.67808
H42	0.729783	3.849549	1.14293
H43	3.321132	2.595109	-1.97063
H44	1.606527	-0.30401	-1.59667
C45	-0.41616	1.096064	-1.07486
H46	0.016044	1.750406	-1.83329
H47	-1.1341	0.414954	-1.55951
H48	-0.9415	1.699279	-0.32792

Table S255. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(\kappa^2\text{-}TFA^{ax,P})$

Atom	x	y	z
Rh1	1.078905	-0.47903	-0.02994
N2	0.279292	-0.30325	2.085021
C3	0.780673	0.724119	2.843634
C4	0.371375	0.90547	4.198802
C5	-0.57473	-0.00784	4.733289

C6	-1.0559	-1.02719	3.947637
C7	-0.59517	-1.14076	2.61582
C8	0.926019	1.972236	4.950885
H9	-0.90237	0.108948	5.762992
H10	-1.77456	-1.74584	4.326525
C11	1.737544	1.616566	2.270329
C12	2.261009	2.637003	3.045307
H13	-0.93874	-1.94063	1.96488
P14	2.250402	1.251578	0.546588
O15	2.106375	-2.53381	0.560861
C16	1.853081	2.818781	4.385873
H17	2.99836	3.311142	2.6221
H18	2.278841	3.630506	4.967582
H19	0.610566	2.106197	5.982287
C20	0.834375	-4.57865	0.370047
C21	1.033111	-3.06131	0.187335
O22	0.044523	-2.42075	-0.28155
F23	-0.04885	-4.78936	1.377059
F24	1.975757	-5.20432	0.685558
F25	0.334396	-5.1449	-0.74033
N26	3.951276	1.052116	0.578867
C27	4.565677	-0.20403	0.641185
C28	5.896046	-0.01315	0.89713
C29	6.123432	1.395414	1.005937
C30	4.924618	2.028276	0.819314
H31	3.985336	-1.10372	0.495009
H32	6.635919	-0.79673	0.984015
H33	7.071123	1.886833	1.181165
H34	4.675017	3.076693	0.780208
N35	2.170285	2.795426	-0.21133
C36	2.758659	3.077454	-1.44596
C37	2.244158	4.258692	-1.91013
C38	1.285981	4.71872	-0.95503
C39	1.243483	3.80452	0.063395
H40	2.530288	4.749549	-2.83006
H41	0.700518	5.626199	-1.00867
H42	0.648338	3.777579	0.961779
H43	3.499031	2.412883	-1.86378
H44	1.678632	-0.51363	-1.45864
C45	-0.36818	0.739037	-0.85678
H46	0.014829	1.452927	-1.5871
H47	-1.02482	0.015111	-1.34862

H48	-0.91488	1.267675	-0.06908

Table S256. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{P})$

Atom	x	y	z
Rh1	0.434422	-0.13583	-0.26938
N2	-0.23346	-0.01182	1.89873
C3	0.504515	0.784306	2.737832
C4	0.178138	0.88959	4.123435
C5	-0.93654	0.149359	4.598357
C6	-1.65312	-0.63857	3.730025
C7	-1.26216	-0.69603	2.372271
C8	0.971942	1.714901	4.960065
H9	-1.20714	0.213724	5.649063
H10	-2.50709	-1.21849	4.063049
C11	1.618657	1.511513	2.214707
C12	2.36779	2.301168	3.07056
H13	-1.78301	-1.31718	1.646945
P14	1.971836	1.271126	0.425896
O15	-0.9707	-1.63846	-0.48473
C16	2.045884	2.404378	4.442734
H17	3.217474	2.856301	2.687485
H18	2.652963	3.033583	5.086141
H19	0.720041	1.791832	6.0143
C20	-2.65327	-3.12617	-1.13175
C21	-1.76638	-1.89675	-1.47134
O22	-1.91122	-1.3251	-2.53786
F23	-3.33452	-2.91223	0.026343
F24	-1.90589	-4.23676	-0.95545
F25	-3.55442	-3.3826	-2.08719
N26	3.608531	0.760646	0.310546
C27	3.965496	-0.56514	0.050167
C28	5.316553	-0.69105	0.225364
C29	5.822759	0.590428	0.609343
C30	4.765876	1.458968	0.661868
H31	3.216933	-1.27604	-0.26775
H32	5.889283	-1.59525	0.074002
H33	6.855892	0.846202	0.801444
H34	4.730175	2.517734	0.86404
N35	2.158631	2.893931	-0.12802
C36	2.738505	3.22382	-1.35501
C37	2.420926	4.523791	-1.64783
C38	1.595623	5.016334	-0.59099

C39	1.433588	4.002931	0.31564
H40	2.753411	5.070245	-2.51952
H41	1.177771	6.009767	-0.50398
H42	0.880955	3.966699	1.24058
H43	3.334881	2.501482	-1.89086
H44	0.986171	-0.23676	-1.71223
C45	-0.67526	1.392897	-1.10544
H46	-0.0576	2.118814	-1.6334
H47	-1.33228	0.856471	-1.78932
H48	-1.2219	1.86432	-0.2835

Table S257. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{P})(TFAH^{ax})$

Atom	x	y	z
Rh1	0.450687	-0.23657	-0.23674
N2	-0.32213	0.162571	1.848274
C3	0.567234	0.741859	2.714929
C4	0.292721	0.803756	4.114003
C5	-0.94089	0.270166	4.57064
C6	-1.81675	-0.2892	3.671461
C7	-1.45864	-0.33188	2.304545
C8	1.25669	1.376838	4.982491
H9	-1.17389	0.30586	5.631656
H10	-2.76504	-0.7097	3.988581
C11	1.790471	1.280022	2.206833
C12	2.703734	1.824206	3.092068
H13	-2.10019	-0.79872	1.561248
P14	2.01506	1.163253	0.385611
O15	-1.26206	-1.46607	-0.61696
C16	2.440979	1.867567	4.480638
H17	3.646354	2.215114	2.725624
H18	3.182553	2.294966	5.148375
H19	1.047915	1.414136	6.048352
C20	-2.71655	-2.94563	-1.71835
C21	-1.28389	-2.52265	-1.30599
O22	-0.34607	-3.24583	-1.69797
F23	-3.2408	-2.03259	-2.56049
F24	-3.51425	-3.00973	-0.63029
F25	-2.74517	-4.13805	-2.32392
N26	3.656118	0.800369	0.05883
C27	4.103859	-0.41494	-0.46729
C28	5.470905	-0.4041	-0.47704
C29	5.898678	0.852523	0.055992

C30	4.780174	1.572823	0.375166
H31	3.394932	-1.14082	-0.82847
H32	6.10072	-1.20299	-0.84253
H33	6.918645	1.193996	0.169317
H34	4.669626	2.58175	0.739708
N35	2.025902	2.826538	-0.07034
C36	2.466223	3.288269	-1.31223
C37	2.052033	4.58514	-1.46226
C38	1.308387	4.939674	-0.29481
C39	1.291644	3.849061	0.533125
H40	2.267495	5.218969	-2.3114
H41	0.849419	5.895694	-0.08361
H42	0.843224	3.707688	1.503504
H43	3.049689	2.650591	-1.95839
H44	1.07957	-0.50051	-1.63051
O45	1.519514	-1.97145	0.958438
C46	2.041392	-2.99877	0.526966
O47	1.804597	-3.61989	-0.5757
C48	3.160321	-3.68062	1.348232
F49	2.81064	-4.93912	1.664875
F50	4.29504	-3.72349	0.626463
F51	3.404588	-3.01123	2.480474
H52	0.912358	-3.30657	-1.07482
C53	-0.57412	1.249943	-1.23557
H54	0.048269	1.822348	-1.924
H55	-1.35812	0.721933	-1.78169
H56	-1.01686	1.918001	-0.49032

Other

Table S258. CH_4

Atom	x	y	z
C1	-1.2E-09	-7.6E-09	-2E-09
H2	0.629885	0.629885	0.629885
H3	-0.62989	-0.62989	0.629885
H4	0.629885	-0.62989	-0.62989
H5	-0.62989	0.629885	-0.62989

Table S259. TFAH

Atom	x	y	z
O1	0	0	0
C2	0	0	1.194706

O3	1.072154	0	1.992513
H4	1.866377	-0.00396	1.435555
C5	-1.29506	-0.01221	2.05074
F6	-1.30318	1.011869	2.920835
F7	-2.36925	0.086168	1.269449
F8	-1.37798	-1.15922	2.749115

Table S260. H_2O

Atom	x	y	z
O1	0	0	0
H2	0	0	0.962495
H3	0.929866	0	-0.24848

Table S261. MeOH

Atom	x	y	z
C1	-1.17235	1.11851	-0.00029
H2	-1.78638	1.777831	0.613746
H3	-1.83758	0.482874	-0.59771
H4	-0.57493	0.482874	0.664946
O5	-0.35832	1.956236	-0.81432
H6	0.197882	1.403732	-1.37052

Table S262. $MeOH_2^+$

Atom	x	y	z
C1	-1.22746	1.097825	0.04028
H2	-1.82504	1.814148	0.595938
H3	-1.82676	0.538295	-0.67159
H4	-0.60132	0.471336	0.669848
O5	-0.31589	1.957273	-0.82589
H6	0.224648	1.471535	-1.47664
H8	0.229295	2.607007	-0.34378

Table S263. CH_3TFA

Atom	x	y	z
O1	0	0	0
C2	0	0	1.197715
O3	1.055591	0	2.002014
C4	2.350226	0.004918	1.354793
C5	-1.30003	0.01049	2.046631
F6	-1.38678	1.150426	2.758643
F7	-2.37212	-0.0751	1.258934
F8	-1.3229	-1.02243	2.908143
H9	2.446987	-0.86788	0.709143

H10	2.466739	0.914613	0.765466
H11	3.073293	-0.02819	2.16504

Table S264. $OVCl_3$

Atom	x	y	z
V1	0	0	0
O2	0	0	1.553381
Cl3	2.036796	0	-0.67365
Cl4	-1.01827	1.763696	-0.67383
Cl5	-1.0192	-1.76316	-0.67382

Table S265. $MeOVCl_3$

Atom	x	y	z
V1	0	0	0
O2	0	0	1.720611
Cl3	2.091485	0	-0.60189
Cl4	-1.08005	1.602679	-0.96133
Cl5	-0.79518	-1.94064	-0.58372
C6	0.540306	-0.78871	2.777224
H7	1.628619	-0.83012	2.686303
H8	0.124152	-1.79809	2.728926
H9	0.261708	-0.31369	3.719785

Tables of Thermodynamic Values

Explanation for column entries

1. Temp: temperature, in Kelvins
2. E_{gas}: gas-phase electronic energies, in hartrees
3. E_{solv}: solution-phase electronic energies, in hartrees
4. G: free energy, as calculated in the Computational Details section, in hartrees
5. ZPE: zero-point energy, in kcal/mol
6. H_{vib}: vibrational enthalpy, in kcal/mol
7. S_{trans}: translational entropy, in cal/mol K
8. S_{rot}: rotational entropy, in cal/mol K
9. S_{vib}: vibrational entropy, in cal/mol K
10. Solv: solvation energy, equal to $E_{solv} - E_{gas}$, in kcal/mol
11. H_{tot}: total enthalpy, in kcal/mol (for gases and pure liquids)
12. S_{tot}: total entropy, in kcal/mol (for gases and pure liquids)
13. $\Delta G_{gas \rightarrow liquid}$: free energy change from gas to liquid, as calculated in the Computational Details section, in kcal/mol (for pure liquids)

Rh(NN) complexes in TFAH

Table S266. $[Rh^{I}(NN)(TFA)(TFAH)]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2004.69	-2004.76	-2004.45	223.525	18.959	45.064	37.742	128.296	-40.5557
498.15	-2004.69	-2004.76	-2004.51	223.525	47.927	47.614	39.272	201.3808	-40.5557

Table S267. $Rh^{I}(NN)(TFAH)_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2005.17	-2005.18	-2004.86	231.973	19.219	45.069	37.726	131.1128	-9.0586
498.15	-2005.17	-2005.18	-2004.93	231.973	48.49	47.619	39.256	204.9532	-9.0586

Table S268. $[Rh^{III}(NN)(TFA)_3(TFAH)^{eq}]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3057.07	-3057.13	-3056.78	261.527	27.536	46.015	38.869	193.4622	-39.0529
498.15	-3057.07	-3057.13	-3056.87	261.527	67.242	48.565	40.399	294.8185	-39.0529

Table S269. $Rh^{III}(NN)(TFA)_2(TFAH^{ax})(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3057.55	-3057.56	-3057.2	267.592	26.878	46.019	38.864	191.6617	-9.88732
498.15	-3057.55	-3057.56	-3057.29	267.592	66.285	48.569	40.394	293.2313	-9.88732

Table S270. $Rh^{III}(NN)(TFA)_2(TFAH^{ax})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3057.54	-3057.56	-3057.2	266.683	26.863	46.019	38.844	191.681	-11.0303
498.15	-3057.54	-3057.56	-3057.29	266.683	66.322	48.569	40.374	293.378	-11.0303

Table S271. $Rh^{III}(NN)(TFA)_2(TFAH^{eq})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3057.55	-3057.56	-3057.2	268.554	27.421	46.019	38.857	192.0941	-10.1498
498.15	-3057.55	-3057.56	-3057.29	268.554	67.159	48.569	40.387	293.5017	-10.1498

Table S272. $[Rh^{III}(NN)(TFA)_2(TFAH^{eq})(CH_3^{ax})]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2570.78	-2570.84	-2570.47	265.301	25.013	45.64	38.302	171.2588	-37.2699
498.15	-2570.78	-2570.84	-2570.56	265.301	61.563	48.19	39.832	263.5718	-37.2699

Table S273. $[Rh^{III}(NN)(TFA)_2(TFAH^{ax})(CH_3^{ax})]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2570.78	-2570.84	-2570.48	266.263	24.455	45.64	38.39	171.496	-38.2609
498.15	-2570.78	-2570.84	-2570.56	266.263	60.546	48.19	39.92	263.661	-38.2609

Table S274. $Rh^{III}(NN)(TFA)(TFAH^{eq})_2(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.26	-2571.27	-2570.89	274.083	24.124	45.644	38.398	173.4274	-7.95737
498.15	-2571.26	-2571.27	-2570.98	274.083	60.041	48.194	39.928	266.1398	-7.95737

Table S275. $Rh^{III}(NN)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.26	-2571.28	-2570.9	274.494	24.57	45.644	38.441	171.9123	-9.3789
498.15	-2571.26	-2571.28	-2570.98	274.494	60.883	48.194	39.971	264.6194	-9.3789

Table S276. $[Rh^{IV}(NN)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571	-2571.06	-2570.68	275.104	24.271	45.644	38.421	168.628	-38.2065
498.15	-2571	-2571.06	-2570.77	275.104	60.603	48.194	39.951	261.3834	-38.2065

Table S277. $Rh^{IV}(NN)(TFA)_2(TFAH^{eq})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2570.62	-2570.64	-2570.28	265.885	24.786	45.64	38.368	168.6428	-14.1673
498.15	-2570.62	-2570.64	-2570.28	265.885	24.786	45.64	38.368	168.6428	-14.1673

Table S278. $Rh^{IV}(NN)(TFA)_2(TFAH^{ax})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2570.63	-2570.66	-2570.29	266.946	24.335	45.64	38.316	169.9426	-15.4495
498.15	-2570.63	-2570.66	-2570.37	266.946	60.42	48.19	39.846	262.0834	-15.4495

Table S279. $Rh^{II}(NN)(TFA)(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2004.59	-2004.6	-2004.29	224.845	18.853	45.064	37.689	128.1089	-11.284
498.15	-2004.59	-2004.6	-2004.36	224.845	47.665	47.614	39.219	200.7931	-11.284

Table S280. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_3^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.22	-2571.24	-2570.86	270.344	23.605	45.644	38.298	168.1886	-9.9754
498.15	-2571.22	-2571.24	-2570.95	270.344	59.39	48.194	39.828	260.5506	-9.9754

Table S281. $[Rh^{III}(NN)(TFA^{eq})(TFAH^{ax})(CH_3^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.22	-2571.24	-2570.86	269.856	24.198	45.644	38.286	168.3633	-10.1621
498.15	-2571.22	-2571.24	-2570.95	269.856	60.429	48.194	39.816	260.8486	-10.1621

Table S282. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.21	-2571.23	-2570.86	270.735	23.647	45.644	38.358	168.4337	-9.4444
498.15	-2571.21	-2571.23	-2570.94	270.735	59.392	48.194	39.888	260.6964	-9.4444

Table S283. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2571.2	-2571.22	-2570.84	271.589	24.156	45.644	38.272	168.3661	-9.48889
498.15	-2571.2	-2571.22	-2570.92	271.589	60.399	48.194	39.802	260.8946	-9.48889

Table S284. $[Rh^{III\text{-}I}(NN)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3097.5	-3097.56	-3097.16	290.463	29.522	46.073	39.426	210.0754	-37.0068
498.15	-3097.5	-3097.56	-3097.26	290.463	71.323	48.623	40.956	316.7253	-37.0068

Table S285. $[Rh^{III\text{-}I}(NN)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFAH)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3097.96	-3097.97	-3097.57	298.763	28.491	46.076	39.458	210.5037	-10.3168
498.15	-3097.96	-3097.97	-3097.67	298.763	69.819	48.626	40.988	317.9511	-10.3168

Table S286. $[Rh^{III\text{-}II}(NN)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4098.54	-4098.56	-4098.19	278.6	30.214	46.274	39.543	216.3189	-16.9192
498.15	-4098.54	-4098.56	-4098.29	278.6	71.682	48.824	41.074	322.2129	-16.9192

Table S287. $[Rh^{IV\text{-}II}(NN)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3097.35	-3097.38	-3096.98	291.79	29.571	46.073	39.279	203.8782	-15.7309
498.15	-3097.35	-3097.38	-3097.07	291.79	71.679	48.623	40.809	310.2941	-15.7309

Table S288. $[Rh^{IV\text{-}II}(NN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3096.89	-3096.95	-3096.57	283.47	29.15	46.069	39.294	205.9239	-38.0829
498.15	-3096.89	-3096.95	-3096.66	283.47	70.7	48.619	40.824	311.9528	-38.0829

Table S289. $[Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH_2TFA^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3096.77	-3096.78	-3096.4	283.819	27.94	46.069	38.974	195.3578	-11.2464
498.15	-3096.77	-3096.78	-3096.49	283.819	68.948	48.619	40.504	299.9599	-11.2464

Table S290. [Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH$_2$TFA^{eq}-H-TFA^{ax})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3096.75	-3096.77	-3096.38	283.981	28.574	46.069	38.927	196.3256	-10.8676
498.15	-3096.75	-3096.77	-3096.47	283.981	69.988	48.619	40.457	300.9533	-10.8676

Table S291. [Rh^{III}(NN)(TFA^{ax})(TFAH^{ax})(CH$_2$TFA^{eq}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3096.75	-3096.76	-3096.38	283.981	28.574	46.069	38.927	196.3256	-11.8248
498.15	-3096.75	-3096.76	-3096.47	283.981	69.988	48.619	40.457	300.9533	-11.8248

Table S292. [Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH$_2$OH^{ax}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2646.43	-2646.45	-2646.07	275.583	22.984	45.708	38.34	166.0769	-12.0654
498.15	-2646.43	-2646.45	-2646.15	275.583	58.857	48.258	39.87	259.6571	-12.0654

Table S293. [Rh^{III}(NN)(TFA^{eq})(TFAH^{ax})(CH$_2$OH^{ax}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2646.43	-2646.45	-2646.07	274.058	24.555	45.708	38.342	170.8068	-12.2809
498.15	-2646.43	-2646.45	-2646.15	274.058	61.404	48.258	39.872	264.85	-12.2809

Table S294. [Rh^{III}(NN)(TFA^{ax})(TFAH^{eq})(CH$_2$OH^{eq}-H-TFA^{ax})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2646.42	-2646.44	-2646.06	274.987	25.204	45.708	38.349	171.6225	-11.118
498.15	-2646.42	-2646.44	-2646.14	274.987	62.464	48.258	39.879	265.7128	-11.118

Table S295. [Rh^{III}(NN)(TFA^{ax})(TFAH^{ax})(CH$_2$OH^{eq}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2646.41	-2646.43	-2646.05	275.126	24.265	45.708	38.365	173.0272	-12.092
498.15	-2646.41	-2646.43	-2646.13	275.126	60.889	48.258	39.895	267.5244	-12.092

Rh(NN^{F}) complexes in TFAH

Table S296. [Rh^{I}(NN^{F})(TFA)(TFAH)]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3493.21	-3493.26	-3493.09	146.152	27.88	46.169	39.481	184.7848	-31.2125
498.15	-3493.21	-3493.26	-3493.18	146.152	65.384	48.72	41.011	279.8869	-31.2125

Table S297. Rh^{I}(NN^{F})(TFAH)$_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3493.67	-3493.69	-3493.5	155.744	27.463	46.173	39.487	186.4464	-9.70394
498.15	-3493.67	-3493.69	-3493.5	155.744	27.463	46.173	39.487	186.4464	-9.70394

Table S298. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})]_2(\mu^2\text{-}TFA^{eq})_2 \cdot 2TFAH$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-9092.08	-9092.1	-9091.63	385.817	74.945	48.926	43.784	520.1435	-11.664
498.15	-9092.08	-9092.1	-9091.85	385.817	173.96	51.476	45.314	774.3644	-11.664

Table S299. $[Rh^{III}(NN^{F})(TFA)_3(TFAH)^{eq}]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4545.57	-4545.62	-4545.4	184.087	36.825	46.857	40.221	247.9255	-33.6463
498.15	-4545.57	-4545.62	-4545.51	184.087	85.379	49.407	41.751	371.0779	-33.6463

Table S300. $[Rh^{III}(NN^{F})(TFA)_3(TFAH)^{ax}]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4545.57	-4545.62	-4545.41	183.025	35.115	46.857	40.213	247.9706	-33.5079
498.15	-4545.57	-4545.62	-4545.52	183.025	82.527	49.407	41.743	371.2424	-33.5079

Table S301. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4546.03	-4546.04	-4545.82	191.213	34.939	46.86	40.262	245.2458	-8.59998
498.15	-4546.03	-4546.04	-4545.93	191.213	82.34	49.41	41.792	368.4665	-8.59998

Table S302. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4546.03	-4546.05	-4545.82	191.178	35.408	46.86	40.251	244.2615	-10.245
498.15	-4546.03	-4546.05	-4545.93	191.178	83.21	49.41	41.781	367.4925	-10.245

Table S303. $Rh^{III}(NN^{F})(TFA)_2(TFAH^{eq})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4546.03	-4546.05	-4545.82	191.245	35.553	46.86	40.245	245.9306	-10.0602
498.15	-4546.03	-4546.05	-4545.93	191.245	83.386	49.41	41.775	369.2456	-10.0602

Table S304. $[Rh^{III}(NN^{F})(TFA)_2(TFAH^{ax})(CH_3{}^{ax})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.29	-4059.35	-4059.12	189.024	33.411	46.578	39.906	228.308	-32.5427
498.15	-4059.29	-4059.35	-4059.22	189.024	78.042	49.128	41.436	342.4968	-32.5427

Table S305. $Rh^{III}(NN^{F})(TFA)(TFAH^{eq})_2(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.75	-4059.76	-4059.52	197.104	33.27	46.581	39.889	225.9873	-7.72411
498.15	-4059.75	-4059.76	-4059.62	197.104	78.03	49.131	41.42	340.4842	-7.72411

Table S306. $Rh^{III}(NN^F)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.76	-4059.77	-4059.53	197.978	33.721	46.581	39.829	225.4284	-7.27421
498.15	-4059.76	-4059.77	-4059.63	197.978	78.915	49.131	41.359	340.023	-7.27421

Table S307. $[Rh^{IV}(NN^F)(TFA)(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.46	-4059.52	-4059.28	197.533	33.028	46.581	39.927	223.826	-38.3963
498.15	-4059.46	-4059.52	-4059.38	197.533	77.846	49.131	41.457	338.4679	-38.3963

Table S308. $Rh^{IV}(NN^F)(TFA)_2(TFAH^{eq})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.09	-4059.11	-4058.88	188.794	32.951	46.578	39.886	223.5947	-12.284
498.15	-4059.09	-4059.11	-4058.99	188.794	77.505	49.128	41.417	337.5756	-12.284

Table S309. $Rh^{IV}(NN^F)(TFA)_2(TFAH^{ax})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.11	-4059.13	-4058.9	189.751	33.149	46.578	39.863	225.8113	-11.8349
498.15	-4059.11	-4059.13	-4059	189.751	77.706	49.128	41.393	339.8042	-11.8349

Table S310. $Rh^{II}(NN^F)(TFA)(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3493.08	-3493.09	-3492.92	147.672	27.668	46.169	39.424	183.4101	-10.9628
498.15	-3493.08	-3493.09	-3493	147.672	64.966	48.72	40.954	277.9857	-10.9628

Table S311. $[Rh^{III}(NN^F)(TFA^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.71	-4059.72	-4059.49	192.832	32.376	46.581	39.858	223.3374	-8.5983
498.15	-4059.71	-4059.72	-4059.59	192.832	76.671	49.131	41.388	337.6476	-8.5983

Table S312. $[Rh^{III}(NN^F)(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.71	-4059.73	-4059.49	193.792	33.369	46.581	39.825	221.607	-9.20221
498.15	-4059.71	-4059.73	-4059.59	193.792	78.409	49.131	41.355	335.7998	-9.20221

Table S313. $[Rh^{III}(NN^F)(TFA^{eq})(TFAH^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.7	-4059.72	-4059.48	193.446	32.865	46.581	39.881	221.8695	-9.10225
498.15	-4059.7	-4059.72	-4059.58	193.446	77.481	49.131	41.411	335.9832	-9.10225

Table S314. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.7	-4059.72	-4059.48	193.687	31.79	46.581	39.894	222.3395	-9.75815
498.15	-4059.7	-4059.72	-4059.59	193.687	75.6	49.131	41.424	336.4275	-9.75815

Table S315. $[Rh^{III}(NN^{F})(TFA^{ax})(TFAH^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4059.68	-4059.7	-4059.46	194.508	33.719	46.581	39.83	224.7544	-11.2469
498.15	-4059.68	-4059.7	-4059.56	194.508	78.983	49.131	41.36	339.5252	-11.2469

Table S316. $[Rh^{III\text{-}I}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4586.01	-4586.06	-4585.8	213.309	37.107	46.9	40.595	264.2832	-31.7924
498.15	-4586.01	-4586.06	-4585.92	213.309	86.624	49.45	42.125	392.8837	-31.7924

Table S317. $[Rh^{III\text{-}I}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFAH)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4586.46	-4586.47	-4586.2	221.132	37.775	46.903	40.671	265.1144	-10.245
498.15	-4586.46	-4586.47	-4586.32	221.132	87.904	49.453	42.201	394.2371	-10.245

Table S318. $[Rh^{III\text{-}II}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-5587.04	-5587.05	-5586.82	202.354	37.479	47.054	40.762	266.3482	-7.77631
498.15	-5587.04	-5587.05	-5586.94	202.354	86.617	49.604	42.292	394.0759	-7.77631

Table S319. $[Rh^{IV\text{-}II}(NN^{F})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.83	-4585.85	-4585.59	214.485	38.382	46.9	40.557	259.1151	-11.204
498.15	-4585.83	-4585.85	-4585.71	214.485	89.031	49.45	42.087	387.5609	-11.204

Table S320. $[Rh^{IV\text{-}II}(NN^{F})(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.38	-4585.44	-4585.19	205.167	38.08	46.898	40.49	261.49	-33.5892
498.15	-4585.38	-4585.44	-4585.31	205.167	88.259	49.448	42.02	389.7751	-33.5892

Table S321. $[Rh^{III}(NN^{F})(TFA^{eq})(TFAH^{ax})(CH_2TFA^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.25	-4585.27	-4585.02	206.712	36.509	46.898	40.357	247.9637	-10.319
498.15	-4585.25	-4585.27	-4585.13	206.712	85.992	49.448	41.887	374.4278	-10.319

Table S322. [$Rh^{III}(NN^F)(TFA^{ax})(TFAH^{eq})(CH_2TFA^{ax}$-H-$TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.25	-4585.26	-4585.01	206.364	37.143	46.898	40.268	248.4888	-10.299
498.15	-4585.25	-4585.26	-4585.12	206.364	87.013	49.448	41.798	374.9172	-10.299

Table S323. [$Rh^{III}(NN^F)(TFA^{eq})(TFAH^{ax})(CH_2TFA^{eq}$-H-$TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.24	-4585.26	-4585.01	206.974	37.156	46.898	40.251	249.0146	-10.0335
498.15	-4585.24	-4585.26	-4585.12	206.974	87.043	49.448	41.781	375.4996	-10.0335

Table S324. [$Rh^{III}(NN^F)(TFA^{ax})(TFAH^{eq})(CH_2TFA^{eq}$-H-$TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.25	-4585.26	-4585.01	206.779	36.81	46.898	40.355	251.0291	-9.48744
498.15	-4585.25	-4585.26	-4585.13	206.779	86.279	49.448	41.885	377.4529	-9.48744

Table S325. [$Rh^{III}(NN^F)(TFA^{ax})(TFAH^{ax})(CH_2TFA^{eq}$-H-$TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4585.23	-4585.25	-4585	207.32	36.894	46.898	40.285	251.4911	-9.85293
498.15	-4585.23	-4585.25	-4585.11	207.32	86.529	49.448	41.815	378.3453	-9.85293

Table S326. [$Rh^{III}(NN^F)(TFA^{eq})(TFAH^{ax})(CH_2OH^{ax}$-H-$TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4134.93	-4134.94	-4134.7	198.209	33.825	46.629	39.88	224.7718	-9.45104
498.15	-4134.93	-4134.94	-4134.8	198.209	79.543	49.179	41.41	340.6763	-9.45104

Table S327. [$Rh^{III}(NN^F)(TFA^{eq})(TFAH^{ax})(CH_2OH^{eq}$-H-$TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4134.9	-4134.92	-4134.68	197.498	32.21	46.629	39.854	224.7499	-10.6838
498.15	-4134.9	-4134.92	-4134.78	197.498	76.784	49.179	41.384	340.7791	-10.6838

Table S328. [$Rh^{III}(NN^F)(TFA^{ax})(TFAH^{eq})(CH_2OH^{eq}$-H-$TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4134.91	-4134.93	-4134.69	197.489	33.446	46.629	39.942	225.9943	-10.5693
498.15	-4134.91	-4134.93	-4134.79	197.489	78.777	49.179	41.472	341.9241	-10.5693

Table S329. [$Rh^{III}(NN^F)(TFA^{ax})(TFAH^{ax})(CH_2OH^{eq}$-H-$TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4134.9	-4134.92	-4134.67	197.942	32.989	46.629	39.881	227.7325	-11.4587
498.15	-4134.9	-4134.92	-4134.78	197.942	78.049	49.179	41.411	343.9895	-11.4587

Rh(NN^F) complexes in H_2O

Table S330. [Rh^I(NN^F)(OH)(H$_2$O)]$^-$·4H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2898.24	-2898.32	-2898.07	193.606	26.405	45.728	38.741	175.716	-49.4247
498.15	-2898.24	-2898.32	-2898.15	193.606	62.834	48.278	40.271	269.1402	-49.4247

Table S331. Rh^I(NN^F)(H$_2$O)$_2$·4H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2898.74	-2898.78	-2898.52	200.758	28.672	45.732	38.444	188.1502	-24.3251
498.15	-2898.74	-2898.78	-2898.61	200.758	66.663	48.282	39.974	284.5957	-24.3251

Table S332. [Rh^{III}(NN^F)(OH)$_3$(H$_2$O^{ax})]$^-$·8H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3355.64	-3355.74	-3355.36	277.787	34.635	46.122	39.242	226.4524	-58.9145
498.15	-3355.64	-3355.74	-3355.47	277.787	81.578	48.672	40.772	345.5563	-58.9145

Table S333. [Rh^{III}(NN^F)(OH)$_3$(H$_2$O^{eq})]$^-$·8H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3355.65	-3355.74	-3355.37	278.268	34.802	46.122	39.174	226.0785	-61.465
498.15	-3355.65	-3355.74	-3355.47	278.268	82.052	48.672	40.704	345.9902	-61.465

Table S334. Rh^{III}(NN^F)(OH)$_2$(H$_2$O^{ax})$_2$·8H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3356.15	-3356.2	-3355.81	287.097	33.799	46.125	39.092	221.6975	-34.4527
498.15	-3356.15	-3356.2	-3355.92	287.097	80.534	48.675	40.622	341.2779	-34.4527

Table S335. Rh^{III}(NN^F)(OH)$_2$(H$_2$O^{ax})(H$_2$O^{eq})·8H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3356.16	-3356.21	-3355.82	287.005	34.545	46.125	39.163	223.6656	-30.9643
498.15	-3356.16	-3356.21	-3355.92	287.005	81.782	48.675	40.694	343.5157	-30.9643

Table S336. Rh^{III}(NN^F)(OH)$_2$(H$_2$O^{eq})$_2$·8H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3356.15	-3356.2	-3355.81	285.759	34.775	46.125	39.211	221.7942	-32.4219
498.15	-3356.15	-3356.2	-3355.92	285.759	82.083	48.675	40.741	346.6477	-32.4219

Table S337. [Rh^{III}(NN^F)(OH)$_2$(H$_2$O^{ax})(CH$_3^{ax}$)]$^-$·6H$_2$O

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.84	-3166.92	-3166.58	258.489	32.401	45.986	39.084	211.9936	-53.6207
498.15	-3166.84	-3166.92	-3166.67	258.489	76.371	48.537	40.614	323.5349	-53.6207

Table S338. $[Rh^{III}(NN^{F})(OH)_2(H_2O^{eq})(CH_3^{ax})]^{-}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.83	-3166.92	-3166.57	260.144	31.767	45.986	39.023	206.0594	-54.132
498.15	-3166.83	-3166.92	-3166.66	260.144	75.448	48.537	40.553	316.8514	-54.132

Table S339. $Rh^{III}(NN^{F})(OH^{ax})(H_2O)_2(CH_3^{ax})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.34	-3167.38	-3167.01	267.929	32.069	45.99	38.877	205.7919	-26.43
498.15	-3167.34	-3167.38	-3167.11	267.929	76.29	48.54	40.407	317.9693	-26.43

Table S340. $Rh^{III}(NN^{F})(OH^{eq})(H_2O)_2(CH_3^{ax})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.35	-3167.39	-3167.03	267.536	32.641	45.99	38.945	210.8959	-27.3467
498.15	-3167.35	-3167.39	-3167.13	267.536	77.231	48.54	40.475	324.0353	-27.3467

Table S341. $Rh^{III}(NN^{F})(OH^{ax})(H_2O)_2(CH_3^{eq})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.34	-3167.39	-3167.03	267.316	32.73	45.99	38.875	212.8359	-26.3418
498.15	-3167.34	-3167.39	-3167.12	267.316	77.277	48.54	40.405	325.8633	-26.3418

Table S342. $Rh^{III}(NN^{F})(OH^{eq})(H_2O)_2(CH_3^{eq})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.34	-3167.39	-3167.03	266.591	32.435	45.99	38.996	215.7371	-32.9096
498.15	-3167.34	-3167.39	-3167.13	266.591	76.634	48.54	40.526	328.8886	-32.9096

Table S343. $[Rh^{IV}(NN^{F})(OH)_3(CH_3^{ax})]^{-}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.18	-3166.26	-3165.93	251.56	31.564	45.983	38.965	204.1332	-54.7603
498.15	-3166.18	-3166.26	-3166.02	251.56	74.953	48.533	40.495	314.1883	-54.7603

Table S344. $Rh^{IV}(NN^{F})(OH)_2(H_2O^{ax})(CH_3^{ax})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.7	-3166.74	-3166.39	260.573	32.603	45.986	38.968	210.6304	-28.8596
498.15	-3166.7	-3166.74	-3166.49	260.573	76.923	48.537	40.498	323.0919	-28.8596

Table S345. $Rh^{IV}(NN^{F})(OH)_2(H_2O^{eq})(CH_3^{ax})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.68	-3166.73	-3166.37	261.076	31.833	45.986	39.012	205.1085	-27.3498
498.15	-3166.68	-3166.73	-3166.47	261.076	75.799	48.537	40.542	316.6393	-27.3498

Table S346. $Rh^{IV}(NN^F)(OH)_2(H_2O^{ax})(CH_3^{eq})\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.7	-3166.74	-3166.39	260.047	32.244	45.986	38.864	209.7574	-25.2573
498.15	-3166.7	-3166.74	-3166.48	260.047	76.213	48.537	40.394	321.3061	-25.2573

Table S347. $[Rh^{II}(NN^F)(OH)_2]^-\cdot 4H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2897.62	-2897.7	-2897.46	186.734	27.28	45.724	38.637	179.5088	-47.3815
498.15	-2897.62	-2897.7	-2897.54	186.734	63.933	48.274	40.167	272.5103	-47.3815

Table S348. $Rh^{II}(NN^F)(OH)(H_2O)\cdot 4H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2898.14	-2898.18	-2897.92	195.535	26.829	45.728	38.691	174.6444	-24.0153
498.15	-2898.14	-2898.18	-2898	195.535	63.527	48.278	40.221	267.738	-24.0153

Table S349. $[Rh^{III}(NN^F)(OH^{ax})(H_2O^{eq})(CH_3^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.28	-3167.33	-3166.97	264.019	31.344	45.99	39.015	206.2794	-26.7195
498.15	-3167.28	-3167.33	-3167.07	264.019	74.935	48.54	40.545	317.8469	-26.7195

Table S350. $[Rh^{III}(NN^F)(OH^{eq})(H_2O^{ax})(CH_3^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.29	-3167.33	-3166.97	265.393	31.527	45.99	39.05	202.7909	-24.2931
498.15	-3167.29	-3167.33	-3167.06	265.393	75.309	48.54	40.581	313.8231	-24.2931

Table S351. $[Rh^{III}(NN^F)(OH)_2(CH_3^{ax}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.77	-3166.86	-3166.52	254.851	31.996	45.986	39.039	207.6416	-54.0891
498.15	-3166.77	-3166.86	-3166.61	254.851	75.74	48.537	40.569	318.6021	-54.0891

Table S352. $[Rh^{III}(NN^F)(OH^{ax})(H_2O^{eq})(CH_3^{eq}\text{-}H\text{-}OH^{ax})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.27	-3167.32	-3166.96	263.304	31.761	45.99	39.024	208.884	-30.7762
498.15	-3167.27	-3167.32	-3167.06	263.304	75.648	48.54	40.554	321.2231	-30.7762

Table S353. $[Rh^{III}(NN^F)(OH^{eq})(H_2O^{ax})(CH_3^{eq}\text{-}H\text{-}OH^{ax})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.28	-3167.32	-3166.96	264.48	32.321	45.99	38.981	209.2267	-26.4462
498.15	-3167.28	-3167.32	-3167.06	264.48	76.63	48.54	40.511	321.6286	-26.4462

Table S354. $[Rh^{III}(NN^{F})(OH)_2(CH_3^{eq}\text{-}H\text{-}OH^{ax})]^{-\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.77	-3166.86	-3166.52	256.155	32.424	45.986	39.03	211.0331	-55.4357
498.15	-3166.77	-3166.86	-3166.62	256.155	76.639	48.537	40.56	323.2134	-55.4357

Table S355. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{ax})(CH_3^{eq}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3167.29	-3167.33	-3166.97	264.574	32.087	45.99	39.007	207.5193	-25.4314
498.15	-3167.29	-3167.33	-3167.07	264.574	76.192	48.54	40.537	319.393	-25.4314

Table S356. $[Rh^{III}(NN^{F})(OH)_2(CH_3^{eq}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3166.76	-3166.85	-3166.51	255.652	32.87	45.986	38.95	214.1084	-56.5363
498.15	-3166.76	-3166.85	-3166.61	255.652	77.294	48.537	40.48	326.8375	-56.5363

Table S357. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 7H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3318.93	-3318.98	-3318.59	284.135	33.805	46.111	39.155	218.8463	-29.2195
498.15	-3318.93	-3318.98	-3318.69	284.135	80.327	48.661	40.685	336.8404	-29.2195

Table S358. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3242.5	-3242.54	-3242.17	268.962	32.035	46.048	39.114	206.1951	-26.1312
498.15	-3242.5	-3242.54	-3242.27	268.962	76.501	48.598	40.644	318.9569	-26.1312

Table S359. $[Rh^{III}(NN^{F})(OH)_2(CH_2OH^{ax}\text{-}H\text{-}OH^{eq})]^{-\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3241.98	-3242.07	-3241.72	258.757	32.194	46.044	39.102	208.6865	-55.7711
498.15	-3241.98	-3242.07	-3241.82	258.757	76.413	48.594	40.632	320.8306	-55.7711

Table S360. $[Rh^{III}(NN^{F})(OH^{eq})(H_2O^{ax})(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3242.5	-3242.54	-3242.17	268.689	32.176	46.048	39.064	207.4214	-24.88
498.15	-3242.5	-3242.54	-3242.27	268.689	76.754	48.598	40.594	320.4731	-24.88

Table S361. $[Rh^{III}(NN^{F})(OH^{ax})(H_2O^{eq})(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{\ddagger}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3242.49	-3242.53	-3242.17	267.683	32.326	46.048	39.078	207.4202	-27.2126
498.15	-3242.49	-3242.53	-3242.27	267.683	77.092	48.598	40.608	320.9596	-27.2126

Table S362. $[Rh^{III}(NN^F)(OH)_2(CH_2OH^{eq}\text{-}H\text{-}OH^{ax})]^{-‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3241.98	-3242.07	-3241.72	260.085	32.085	46.044	39.123	212.6428	-56.7538
498.15	-3241.98	-3242.07	-3241.82	260.085	76.32	48.594	40.653	325.8575	-56.7538

Table S363. $[Rh^{III}(NN^F)(OH^{ax})(H_2O^{ax})(CH_2OH^{eq}\text{-}H\text{-}OH^{eq})]^{‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3242.5	-3242.54	-3242.18	268.371	32.42	46.048	39.097	209.9233	-26.6478
498.15	-3242.5	-3242.54	-3242.28	268.371	77.074	48.598	40.627	323.1714	-26.6478

Table S364. $[Rh^{III}(NN^F)(OH)_2(CH_2OH^{eq}\text{-}H\text{-}OH^{eq})]^{-‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3241.98	-3242.07	-3241.73	259.341	33.087	46.044	39.027	216.0679	-56.7744
498.15	-3241.98	-3242.07	-3241.83	259.341	77.986	48.594	40.557	329.9784	-56.7744

Table S365. $[Rh^{III\text{-}I}(NN^F)(OH^{eq})(H_2O)_2(CH_3{}^{ax}\text{-}OH_2)]^{‡}\cdot 7H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3320.13	-3320.19	-3319.78	298.439	34.909	46.118	39.371	232.1926	-34.7761
498.15	-3320.13	-3320.19	-3319.89	298.439	82.359	48.668	40.901	353.5906	-34.7761

Table S366. $[Rh^{III\text{-}I}(NN^F)(OH^{eq})_2(H_2O^{ax})(CH_3{}^{ax}\text{-}OH_2)]^{-‡}\cdot 8H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3396.05	-3396.15	-3395.74	304.74	36.542	46.177	39.522	244.9541	-61.6865
498.15	-3396.05	-3396.15	-3395.85	304.74	85.482	48.727	41.053	370.1436	-61.6865

Table S367. $[Rh^{III\text{-}II}(NN^F)(OH^{ax})(H_2O^{eq})_2(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4694.63	-4694.67	-4694.31	272.502	37.758	46.557	40.065	249.4057	-28.3585
498.15	-4694.63	-4694.67	-4694.43	272.502	87.192	49.107	41.595	374.9201	-28.3585

Table S368. $[Rh^{III\text{-}II}(NN^F)(OH^{eq})(H_2O)_2(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4694.63	-4694.68	-4694.32	272.452	37.756	46.557	39.934	249.2814	-29.4176
498.15	-4694.63	-4694.68	-4694.43	272.452	87.35	49.107	41.464	375.2083	-29.4176

Table S369. $[Rh^{III\text{-}II}(NN^F)(OH^{eq})_2(H_2O^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{-‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4694.13	-4694.21	-4693.87	263.535	37.375	46.554	40.031	254.3423	-52.9534
498.15	-4694.13	-4694.21	-4693.98	263.535	85.934	49.104	41.561	378.6405	-52.9534

Table S370. $[Rh^{III\text{-}II}(NN^{F})(OH)_2(H_2O^{eq})(CH_3^{ax}\text{-}OVCl_3)]^{-‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4694.14	-4694.21	-4693.87	265.362	37.224	46.554	40.081	246.6785	-49.015
498.15	-4694.14	-4694.21	-4693.98	265.362	86.095	49.104	41.611	370.7448	-49.015

Table S371. $[Rh^{IV\text{-}II}(NN^{F})(OH^{eq})_2(H_2O^{ax})(CH_3^{ax}\text{-}OH_2)]^{‡}\cdot 6H_2O$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3243.08	-3243.13	-3242.76	276.47	33.018	46.051	39.149	214.7101	-30.7229
498.15	-3243.08	-3243.13	-3242.86	276.47	78.235	48.601	40.679	329.4021	-30.7229

Rh(ONN) complexes in TFAH

Table S372. $[Rh^{I}(ONN)(TFA)]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1475.78	-1475.86	-1475.61	180.529	13.498	44.375	36.17	87.05742	-50.6518
498.15	-1475.78	-1475.86	-1475.66	180.529	35.469	46.925	37.7	142.4571	-50.6518

Table S373. $Rh^{I}(ONN)(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1476.3	-1476.31	-1476.05	188.555	13.405	44.381	36.254	86.56158	-10.012
498.15	-1476.3	-1476.31	-1476.09	188.555	35.467	46.931	37.784	142.167	-10.012

Table S374. $[Rh^{III}(ONN)(TFA)_3]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2528.14	-2528.22	-2527.92	217.454	22.594	45.531	37.855	151.7098	-46.1476
498.15	-2528.14	-2528.22	-2528	217.454	55.728	48.081	39.385	235.4498	-46.1476

Table S375. $Rh^{III}(ONN)(TFA)_2(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2528.63	-2528.66	-2528.35	225.817	22.171	45.535	37.821	148.2837	-17.027
498.15	-2528.63	-2528.66	-2528.42	225.817	55.353	48.085	39.351	232.1177	-17.027

Table S376. $Rh^{III}(ONN)(TFA)_2(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2528.64	-2528.66	-2528.36	225.412	21.791	45.535	37.864	149.6279	-15.2573
498.15	-2528.64	-2528.66	-2528.43	225.412	54.581	48.085	39.394	233.4745	-15.2573

Table S377. $[Rh^{III}(ONN)(TFA)_2(CH_3^{ax})]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2041.84	-2041.92	-2041.62	221.859	19.139	45.084	37.127	131.5477	-49.9229
498.15	-2041.84	-2041.92	-2041.68	221.859	48.366	47.634	38.657	206.4184	-49.9229

Table S378. $Rh^{III}(ONN)(TFA)(TFAH^{ax})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2042.36	-2042.38	-2042.06	230.076	18.88	45.089	37.194	128.7357	-13.8482
498.15	-2042.36	-2042.38	-2042.13	230.076	48.122	47.639	38.724	203.559	-13.8482

Table S379. $Rh^{III}(ONN)(TFA)(TFAH^{eq})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2042.36	-2042.38	-2042.06	229.941	18.933	45.089	37.144	130.0095	-13.5523
498.15	-2042.36	-2042.38	-2042.13	229.941	48.185	47.639	38.674	204.8588	-13.5523

Table 380. $Rh^{II}(ONN)(TFA)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1475.67	-1475.7	-1475.45	181.826	13.292	44.375	35.988	85.31709	-19.7987
498.15	-1475.67	-1475.7	-1475.5	181.826	35.12	46.925	37.518	140.3923	-19.7987

Table 381. $[Rh^{III}(ONN)(TFA^{ax})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2042.3	-2042.33	-2042.01	227.507	19.169	45.089	37.128	126.5272	-15.9433
498.15	-2042.3	-2042.33	-2042.08	227.507	48.763	47.639	38.658	201.2367	-15.9433

Table 382. $[Rh^{III}(ONN)(TFA^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2042.31	-2042.33	-2042.01	227.589	19.094	45.089	37.143	125.2782	-14.3715
498.15	-2042.31	-2042.33	-2042.08	227.589	48.651	47.639	38.673	199.8916	-14.3715

Table 383. $[Rh^{III\text{-}I}(ONN)(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2568.6	-2568.67	-2568.33	246.713	23.98	45.598	38.527	168.2421	-43.0139
498.15	-2568.6	-2568.67	-2568.42	246.713	58.736	48.148	40.057	257.0757	-43.0139

Table 384. $[Rh^{III\text{-}II}(ONN)(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3569.64	-3569.66	-3569.35	233.947	24.486	45.833	38.73	175.6166	-13.3111
498.15	-3569.64	-3569.66	-3569.43	233.947	58.92	48.383	40.26	264.734	-13.3111

Table 385. $[Rh^{I\text{-}III}(ONN)(H)(CH_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-989.96	-989.98	-989.706	190.281	10.483	43.698	34.572	65.2412	-12.8956
498.15	-989.96	-989.98	-989.745	190.281	29.072	46.248	36.102	112.027	-12.8956

Rh(ONN^{F}) complexes in TFAH

Table 386. [Rh^{I}(ONN^{F})(TFA)]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1971.95	-1972.03	-1971.82	154.816	16.459	44.89	36.962	106.3635	-47.6887
498.15	-1971.95	-1972.03	-1971.88	154.816	41.285	47.44	38.492	169.1293	-47.6887

Table 387. Rh^{I}(ONN^{F})(TFAH)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1972.46	-1972.48	-1972.26	163.051	16.276	44.895	37.161	104.1869	-9.5353
498.15	-1972.46	-1972.48	-1972.31	163.051	41.151	47.445	38.691	167.0484	-9.5353

Table 388. [Rh^{III}(ONN^{F})(TFA)$_3$]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3024.31	-3024.39	-3024.14	191.773	25.505	45.89	38.421	170.5877	-45.85
498.15	-3024.31	-3024.39	-3024.22	191.773	61.467	48.44	39.951	261.625	-45.85

Table 389. Rh^{III}(ONN^{F})(TFA)$_2$(TFAH^{eq})

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3024.8	-3024.83	-3024.56	199.74	24.662	45.894	38.484	167.1812	-16.6718
498.15	-3024.8	-3024.83	-3024.65	199.74	60.27	48.444	40.014	258.2992	-16.6718

Table 390. [Rh^{III}(ONN^{F})(TFA)$_2$(CH$_3^{ax}$)]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2538.01	-2538.09	-2537.83	196.475	21.368	45.497	37.77	148.897	-46.7909
498.15	-2538.01	-2538.09	-2537.9	196.475	52.997	48.047	39.3	230.9295	-46.7909

Table 391. Rh^{III}(ONN^{F})(TFA)(TFAH^{ax})(CH$_3^{ax}$)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2538.53	-2538.55	-2538.28	204.769	21.705	45.501	37.875	146.3524	-14.0428
498.15	-2538.53	-2538.55	-2538.35	204.769	53.761	48.051	39.405	228.4362	-14.0428

Table 392. Rh^{II}(ONN^{F})(TFA)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1971.83	-1971.87	-1971.66	156.122	16.204	44.89	36.923	103.5521	-20.6616
498.15	-1971.83	-1971.87	-1971.71	156.122	40.858	47.44	38.453	165.8749	-20.6616

Table 393. [Rh^{III}(ONN^{F})(TFA^{ax})(CH$_3^{ax}$-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2538.46	-2538.49	-2538.22	201.793	21.545	45.501	37.851	145.0444	-17.3724
498.15	-2538.46	-2538.49	-2538.29	201.793	53.552	48.051	39.381	227.0039	-17.3724

Table 394. $[Rh^{III}(ONN^{F})(TFA^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2538.47	-2538.49	-2538.22	201.867	20.835	45.501	37.91	143.02	-14.9222
498.15	-2538.47	-2538.49	-2538.29	201.867	52.435	48.051	39.44	224.952	-14.9222

Table 395. $[Rh^{III\text{-}I}(ONN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3064.76	-3064.83	-3064.54	221.027	25.796	45.95	39.099	186.7083	-44.5034
498.15	-3064.76	-3064.83	-3064.63	221.027	62.658	48.5	40.629	283.0238	-44.5034

Table 396. $[Rh^{III\text{-}II}(ONN^{F})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4065.81	-4065.83	-4065.56	208.931	27.172	46.159	39.158	186.7871	-14.1193
498.15	-4065.81	-4065.83	-4065.65	208.931	64.387	48.709	40.688	282.062	-14.1193

Rh(ONN^{NMe2}) complexes in TFAH

Table 397. $[Rh^{I}(ONN^{NMe2})(TFA)]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1609.69	-1609.77	-1609.45	226.436	16.095	44.633	44.633	103.9382	-51.4615
498.15	-1609.69	-1609.77	-1609.5	226.436	41.801	47.183	38.397	168.7678	-51.4615

Table 398. $Rh^{I}(ONN^{NMe2})(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1610.2	-1610.22	-1609.88	234.529	16.006	44.638	36.935	103.3847	-10.5782
498.15	-1610.2	-1610.22	-1609.94	234.529	41.819	47.188	38.466	168.4604	-10.5782

Table 399. $[Rh^{III}(ONN^{NMe2})(TFA)_3]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2662.05	-2662.13	-2661.76	263.407	24.641	45.708	38.351	168.0773	-47.7641
498.15	-2662.05	-2662.13	-2661.85	263.407	61.126	48.258	39.881	261.277	-47.7641

Table S400. $Rh^{III}(ONN^{NMe2})(TFA)_2(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2662.54	-2662.57	-2662.19	271.718	24.92	45.712	38.335	166.2829	-18.0247
498.15	-2662.54	-2662.57	-2662.27	271.718	61.879	48.262	39.865	259.6552	-18.0247

Table S401. $Rh^{III}(ONN^{NMe2})(TFA)_2(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2662.55	-2662.58	-2662.2	271.359	24.531	45.712	38.36	167.7531	-16.2924
498.15	-2662.55	-2662.58	-2662.28	271.359	61.101	48.262	39.89	261.1458	-16.2924

Table S402. $[Rh^{III}(ONN^{HNMe_2})(TFA)_2(TFAH^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2662.48	-2662.55	-2662.17	272.369	25.331	45.712	38.333	169.5961	-46.5037
498.15	-2662.48	-2662.55	-2662.25	272.369	62.467	48.262	39.863	263.4273	-46.5037

Table S403. $[Rh^{III}(ONN^{NMe_2})(TFA)_2(CH_3^{ax})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2175.75	-2175.83	-2175.45	267.824	21.744	45.289	37.706	148.3071	-51.3509
498.15	-2175.75	-2175.83	-2175.53	267.824	54.717	47.839	39.236	232.5741	-51.3509

Table S404. $Rh^{III}(ONN^{NMe_2})(TFA)(TFAH^{ax})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2176.27	-2176.29	-2175.9	276.084	22.115	45.293	37.76	146.0812	-14.5163
498.15	-2176.27	-2176.29	-2175.98	276.084	55.518	47.843	39.29	230.407	-14.5163

Table S405. $Rh^{III}(ONN^{NMe_2})(TFA)(TFAH^{eq})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2176.27	-2176.29	-2175.9	276.124	22.082	45.293	37.739	145.8006	-14.4041
498.15	-2176.27	-2176.29	-2175.98	276.124	55.48	47.843	39.269	230.1151	-14.4041

Table S406. $Rh^{II}(ONN^{NMe_2})(TFA)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1609.58	-1609.61	-1609.29	227.822	15.962	44.633	36.729	102.7922	-20.4248
498.15	-1609.58	-1609.61	-1609.34	227.822	41.556	47.183	38.259	167.3376	-20.4248

Table S407. $[Rh^{III}(ONN^{NMe_2})(TFA^{ax})(CH_3^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2176.21	-2176.24	-2175.85	273.485	21.884	45.293	37.696	144.1964	-16.0518
498.15	-2176.21	-2176.24	-2175.92	273.485	55.25	47.843	39.227	228.4332	-16.0518

Table S408. $[Rh^{III}(ONN^{NMe_2})(TFA^{ax})(CH_3^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2176.21	-2176.24	-2175.85	273.586	21.778	45.293	37.722	142.9036	-14.6634
498.15	-2176.21	-2176.24	-2175.92	273.586	55.108	47.843	39.253	227.0438	-14.6634

Table S409. $[Rh^{III\text{-}I}(ONN^{NMe_2})(TFA^{eq})(TFAH^{ax})(CH_3^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2702.51	-2702.57	-2702.17	292.74	27.027	45.772	38.904	184.018	-42.785
498.15	-2702.51	-2702.57	-2702.26	292.74	65.936	48.322	40.434	282.3364	-42.785

Table S410. $[Rh^{III\text{-}II}(ONN^{NMe2})(TFA^{eq})(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3703.55	-3703.58	-3703.2	280.476	27.21	45.993	39.135	189.2617	-21.4258
498.15	-3703.55	-3703.58	-3703.29	280.476	65.383	48.543	40.665	286.8085	-21.4258

Rh(DPMS) complexes in TFAH

Table S411. $[Rh^{I}(DPMS)(TFA)(TFAH)]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2320.28	-2320.37	-2320.15	162.46	16.337	44.952	36.997	112.5266	-53.1868
498.15	-2320.28	-2320.37	-2320.21	162.46	40.938	47.502	38.528	175.6853	-53.1868

Table S412. $Rh^{I}(DPMS)(TFAH)_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2320.78	-2320.81	-2320.58	171.529	16.105	44.958	36.757	109.8819	-17.8001
498.15	-2320.78	-2320.81	-2320.64	171.529	40.807	47.508	38.287	173.2851	-17.8001

Table S413. $[Rh^{III}(DPMS)(TFA)_3(TFAH^{eq})]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3372.63	-3372.71	-3372.45	200.043	25.639	45.935	38.419	172.7861	-49.7837
498.15	-3372.63	-3372.71	-3372.54	200.043	61.743	48.485	39.949	264.1465	-49.7837

Table S414. $[Rh^{III}(DPMS)(TFA)_3]^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2845.86	-2845.95	-2845.72	175.534	20.395	45.479	37.556	139.8423	-54.2072
498.15	-2845.86	-2845.95	-2845.79	175.534	50.206	48.03	39.086	216.2434	-54.2072

Table S415. $Rh^{III}(DPMS)(TFA)_2(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2846.33	-2846.37	-2846.13	183.245	20.221	45.484	37.548	138.7175	-25.4426
498.15	-2846.33	-2846.37	-2846.2	183.245	50.193	48.034	39.078	215.5105	-25.4426

Table S416. $Rh^{III}(DPMS)(TFA)_2(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2846.35	-2846.39	-2846.14	183.312	20.774	45.484	37.549	138.2371	-23.7559
498.15	-2846.35	-2846.39	-2846.21	183.312	51.069	48.034	39.079	214.8349	-23.7559

Table S417. $[Rh^{III}(DPMS)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})]^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2846.7	-2846.78	-2846.53	191.432	20.799	45.488	37.592	137.8329	-50.4104
498.15	-2846.7	-2846.78	-2846.59	191.432	51.348	48.038	39.122	215.0604	-50.4104

Table S418. $[Rh^{III}(DPMS)(TFA^{ax})(TFAH^{eq})_2]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2846.69	-2846.78	-2846.53	191.223	20.513	45.488	37.575	140.7724	-54.9128
498.15	-2846.69	-2846.78	-2846.6	191.223	50.83	48.038	39.105	218.428	-54.9128

Table S419. $Rh^{III}(DPMS)(TFA^{eq})_2(TFAH^{ax})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3373.09	-3373.13	-3372.85	209.236	25.476	45.938	38.359	170.9622	-22.2986
498.15	-3373.09	-3373.13	-3372.93	209.236	61.79	48.488	39.889	262.843	-22.2986

Table S420. $Rh^{III}(DPMS)(TFA^{ax})(TFA^{eq})(TFAH^{ax})(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3373.1	-3373.14	-3372.86	208.68	25.432	45.938	38.37	170.4106	-23.3401
498.15	-3373.1	-3373.14	-3372.94	208.68	61.641	48.488	39.9	262.0172	-23.3401

Table S421. $Rh^{III}(DPMS)(TFA^{ax})_2(TFAH^{eq})_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3373.08	-3373.12	-3372.84	208.411	25.661	45.938	38.4	173.2836	-25.0328
498.15	-3373.08	-3373.12	-3372.93	208.411	62.001	48.488	39.93	265.2363	-25.0328

Table S422. $[Rh^{III}(DPMS)(TFA^{ax})_2(TFAH^{eq})(CH_3{}^{ax})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2886.34	-2886.41	-2886.14	204.981	22.763	45.548	37.957	152.5254	-47.6465
498.15	-2886.34	-2886.41	-2886.21	204.981	55.383	48.098	39.487	235.023	-47.6465

Table S423. $Rh^{III}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.08	-2360.11	-2359.86	187.57	16.564	45.029	36.732	115.4591	-22.8019
498.15	-2360.08	-2360.11	-2359.92	187.57	42.543	47.579	38.262	183.0935	-22.8019

Table S424. $[Rh^{III}(DPMS)(TFAH^{eq})_2(CH_3{}^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.62	-2360.69	-2360.42	196.579	17.381	45.034	36.778	117.1315	-44.1069
498.15	-2360.62	-2360.69	-2360.48	196.579	44.124	47.584	38.308	185.6949	-44.1069

Table S425. $Rh^{III}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.06	-2360.09	-2359.84	187.943	17.328	45.029	36.898	118.1679	-21.2164
498.15	-2360.06	-2360.09	-2359.9	187.943	43.723	47.579	38.428	185.8601	-21.2164

Table S426. $[Rh^{IV}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.76	-2359.83	-2359.58	188.182	17.377	45.029	36.855	117.9892	-49.9776
498.15	-2359.76	-2359.83	-2359.64	188.182	43.867	47.579	38.385	185.9278	-49.9776

Table S427. $[Rh^{IV}(DPMS)(TFA^{eq})(TFAH^{eq})(CH_3^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.76	-2359.85	-2359.59	187.749	17.198	45.029	36.74	115.1683	-53.0999
498.15	-2359.76	-2359.85	-2359.65	187.749	43.682	47.579	38.27	183.0884	-53.0999

Table S428. $Rh^{IV}(DPMS)(TFA)_2(CH_3^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.39	-2359.43	-2359.19	180.469	17.459	45.024	36.769	119.7783	-24.6163
498.15	-2359.39	-2359.43	-2359.25	180.469	43.768	47.574	38.299	187.2728	-24.6163

Table S429. $Rh^{IV}(DPMS)(TFA)_2(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.37	-2359.41	-2359.17	180.474	17.279	45.024	36.719	117.1867	-22.6544
498.15	-2359.37	-2359.41	-2359.23	180.474	43.545	47.574	38.249	184.5682	-22.6544

Table S430. $Rh^{II}(DPMS)(TFA)(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2320.17	-2320.21	-2319.99	163.879	15.957	44.952	36.706	108.9615	-25.3087
498.15	-2320.17	-2320.21	-2320.05	163.879	40.369	47.502	38.236	171.6361	-25.3087

Table S431. $[Rh^{III}(DPMS)(TFA^{eq})(CH_3^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.01	-2360.05	-2359.8	185.193	17.695	45.029	36.738	115.999	-27.2785
498.15	-2360.01	-2360.05	-2359.86	185.193	44.478	47.579	38.268	183.67	-27.2785

Table S432. $[Rh^{III}(DPMS)(TFAH^{eq})(CH_3^{ax}\text{-}H\text{-}TFA^{eq})]^{+‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.38	-2360.46	-2360.2	193.387	17.552	45.034	36.788	113.8006	-52.2835
498.15	-2360.38	-2360.46	-2360.26	193.387	44.45	47.584	38.318	181.7392	-52.2835

Table S433. $[Rh^{III}(DPMS)(TFA^{eq})(CH_3^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.02	-2360.05	-2359.8	185.351	17.57	45.029	36.76	115.2417	-24.5552
498.15	-2360.02	-2360.05	-2359.86	185.351	44.293	47.579	38.29	182.7505	-24.5552

Table S434. [Rh^{III}(DPMS)(TFA^{ax})(CH$_3^{eq}$-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.02	-2360.06	-2359.81	185.394	17.596	45.029	36.763	115.2254	-24.3028
498.15	-2360.02	-2360.06	-2359.87	185.394	44.331	47.579	38.293	182.769	-24.3028

Table S435. [Rh^{III}(DPMS)(TFAH^{eq})(CH$_3^{eq}$-H-TFA^{ax})]$^{+‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.38	-2360.46	-2360.2	193.166	17.675	45.034	36.779	115.5222	-49.8898
498.15	-2360.38	-2360.46	-2360.26	193.166	44.589	47.584	38.309	183.5025	-49.8898

Table S436. [Rh^{III-I}(DPMS)(TFA^{eq})(TFAH^{eq})(CH$_3^{ax}$-TFA)]$^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2886.31	-2886.39	-2886.12	204.113	21.777	45.548	38.325	156.0772	-51.2524
498.15	-2886.31	-2886.39	-2886.2	204.113	53.276	48.098	39.855	237.7411	-51.2524

Table S437. [Rh^{III-II}(DPMS)(TFA^{eq})(TFAH^{eq})(CH$_3^{ax}$-OVCl$_3$)]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3887.35	-3887.39	-3887.14	192.011	21.614	45.786	38.51	158.1071	-22.5196
498.15	-3887.35	-3887.39	-3887.22	192.011	52.368	48.336	40.04	238.9709	-22.5196

Table S438. [Rh^{IV-II}(DPMS)(TFA^{eq})(TFAH^{eq})(CH$_3^{ax}$-TFA)]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2886.15	-2886.19	-2885.91	205.677	21.424	45.548	38.186	146.3765	-25.2402
498.15	-2886.15	-2886.19	-2885.99	205.677	53.087	48.098	39.716	227.4401	-25.2402

Table S439. [Rh^{IV-II}(DPMS)(TFA)$_2$(CH$_3^{ax}$-TFA)]$^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.67	-2885.75	-2885.49	197.234	21.821	45.544	38.189	150.1202	-53.1358
498.15	-2885.67	-2885.75	-2885.56	197.234	53.503	48.094	39.719	231.2583	-53.1358

Table S440. [Rh^{III}(DPMS)(TFA^{eq})(CH$_2$TFA^{ax}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.55	-2885.59	-2885.32	198.425	21.374	45.544	37.723	142.2832	-27.1282
498.15	-2885.55	-2885.59	-2885.4	198.425	52.966	48.094	39.253	222.1482	-27.1282

Table S441. [Rh^{III}(DPMS)(TFA^{eq})(CH$_2$TFA^{eq}-H-TFA^{ax})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.56	-2885.6	-2885.33	198.367	21.349	45.544	37.719	142.0684	-25.9637
498.15	-2885.56	-2885.6	-2885.4	198.367	52.931	48.094	39.249	221.9014	-25.9637

Table S442. [Rh^{III}(DPMS)(TFA^{ax})(CH$_2$TFA^{eq}-H-TFA^{eq})]‡

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.57	-2885.61	-2885.34	198.276	20.855	45.544	37.749	142.745	-24.2056
498.15	-2885.57	-2885.61	-2885.41	198.276	52.071	48.094	39.279	222.6584	-24.2056

Table S443. [Rh^{I-III}(DPMS)(H)(CH$_3$)(TFA^{eq})]$^{-‡}$ (no assisted deprotonation; H cis to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.95	-1834.04	-1833.81	165.897	13.865	44.4	35.937	91.07005	-55.9773
498.15	-1833.95	-1834.04	-1833.86	165.897	35.26	46.95	37.467	145.078	-55.9773

Table S444. [Rh^{I-III}(DPMS)(H)(CH$_3$)(TFA^{eq})]$^{-‡}$ (no assisted deprotonation; H trans to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.96	-1834.05	-1833.82	165.964	13.879	44.4	35.834	91.94615	-55.4296
498.15	-1833.96	-1834.05	-1833.87	165.964	35.231	46.95	37.364	145.8441	-55.4296

Table S445. [Rh^{I-III}(DPMS)(CH$_3$)(H-TFA^{eq})]$^{-‡}$ (TFA^{eq} assisted deprotonation; H cis to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.93	-1834.01	-1833.78	165.371	13.619	44.4	35.844	88.48304	-53.6149
498.15	-1833.93	-1834.01	-1833.83	165.371	34.967	46.95	37.374	142.3614	-53.6149

Table S446. [Rh^{I-III}(DPMS)(H)(CH$_3$)(TFAH^{eq})]‡ (no assisted deprotonation; H cis to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1834.46	-1834.49	-1834.25	173.406	13.602	44.406	35.596	87.88735	-18.4773
498.15	-1834.46	-1834.49	-1834.3	173.406	35.106	46.956	37.126	142.1485	-18.4773

Table S447. [Rh^{I-III}(DPMS)(H)(CH$_3$)(TFAH^{eq})]‡ (no assisted deprotonation; H trans to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1834.46	-1834.49	-1834.25	173.207	13.021	44.406	35.588	87.84133	-18.3978
498.15	-1834.46	-1834.49	-1834.3	173.207	34.066	46.956	37.118	141.9438	-18.3978

Table S448. [Rh^{I-III}(DPMS)(H-TFA)(CH$_3$)(TFAH^{eq})]$^{-‡}$ (unbound TFA deprotonation; H trans to sulfonate)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.72	-2360.8	-2360.55	188.648	18.018	45.034	37.122	124.0078	-48.8009
498.15	-2360.72	-2360.8	-2360.61	188.648	44.96	47.584	38.652	193.0867	-48.8009

Table S449. Rh^{III}(DPMS)(H^{ax})(CH$_3$^{eq})(TFAH^{eq})

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1834.48	-1834.51	-1834.26	174.968	13.627	44.406	35.605	88.55607	-17.7564
498.15	-1834.48	-1834.51	-1834.31	174.968	35.265	46.956	37.135	143.1469	-17.7564

Table S450. $Rh^{III}(DPMS)(H^{eq})(CH_3{}^{ax})(TFAH^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1834.48	-1834.51	-1834.26	175.062	13.606	44.406	35.612	88.22883	-18.4522
498.15	-1834.48	-1834.51	-1834.31	175.062	35.206	46.956	37.142	142.7197	-18.4522

Table S451. $[Rh^{I}(DPMS)(TFAH)(CH_3)]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.95	-1834.03	-1833.8	166.64	13.719	44.4	35.657	89.18497	-50.0136
498.15	-1833.95	-1834.03	-1833.85	166.64	35.241	46.95	37.187	143.5042	-50.0136

Table S452. $[Rh^{III}(DPMS)(TFAH^{eq})(CH_3{}^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.61	-1833.69	-1833.45	170.454	13.417	44.4	35.558	86.38962	-51.2662
498.15	-1833.61	-1833.69	-1833.5	170.454	34.677	46.95	37.088	140.0403	-51.2662

Table S453. $Rh^{III}(DPMS)(TFA^{eq})(CH_3{}^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.23	-1833.28	-1833.05	162.314	13.435	44.393	35.59	87.24738	-27.5976
498.15	-1833.23	-1833.28	-1833.1	162.314	34.497	46.944	37.12	140.4134	-27.5976

Table S454. $Rh^{III}(DPMS)(TFA^{ax})(TFAH^{eq})(CH_3{}^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.06	-2360.09	-2359.84	187.943	17.328	45.029	36.898	118.1679	-21.2164
498.15	-2360.06	-2360.09	-2359.9	187.943	43.723	47.579	38.428	185.8601	-21.2164

Table S455. $[Rh^{IV}(DPMS)(TFA^{eq})(CH_3{}^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1832.93	-1833.02	-1832.8	162.159	12.875	44.393	35.344	86.50673	-59.0053
498.15	-1832.93	-1833.02	-1832.85	162.159	33.629	46.944	36.874	139.899	-59.0053

Table S456. $[Rh^{II}(DPMS)(TFA^{eq})(CH_3{}^{eq})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.36	-1833.45	-1833.23	160.991	13.84	44.393	35.76	90.99446	-57.522
498.15	-1833.36	-1833.45	-1833.28	160.991	35.049	46.944	37.29	144.5404	-57.522

Table S457. $Rh^{II}(DPMS)(TFAH^{eq})(CH_3{}^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1833.87	-1833.9	-1833.67	168.95	13.585	44.4	35.613	87.893	-20.0167
498.15	-1833.87	-1833.9	-1833.71	168.95	34.879	46.95	37.143	141.6338	-20.0167

Rh(DPES) complexes in TFAH

Table S458. [Rh^{I}(DPES)(TFA)(TFAH)]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.56	-2359.65	-2359.4	180.327	17.052	45.024	36.978	116.3253	-50.8097
498.15	-2359.56	-2359.65	-2359.46	180.327	43.086	47.574	38.508	183.101	-50.8097

Table S459. Rh^{I}(DPES)(TFAH)$_2$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2360.07	-2360.09	-2359.83	189.416	17.404	45.029	36.88	113.856	-17.0705
498.15	-2360.07	-2360.09	-2359.89	189.416	43.96	47.579	38.41	180.9316	-17.0705

Table S460. [Rh^{III}(DPES)(TFA)$_3$]$^{-}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.15	-2885.24	-2884.98	193.354	21.682	45.539	37.662	143.3178	-53.4706
498.15	-2885.15	-2885.24	-2885.05	193.354	53.337	48.089	39.192	223.3725	-53.4706

Table S461. Rh^{III}(DPES)(TFA)$_2$(TFAH^{eq})

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2885.64	-2885.68	-2885.41	200.16	20.441	45.544	37.674	142.5948	-23.3833
498.15	-2885.64	-2885.68	-2885.48	200.16	51.456	48.094	39.204	223.0101	-23.3833

Table S462. [Rh^{III}(DPES)(TFA^{eq})(TFAH^{ax})(TFAH^{eq})]$^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2886	-2886.08	-2885.8	208.914	21.043	45.548	37.673	142.5163	-50.5163
498.15	-2886	-2886.08	-2885.87	208.914	52.628	48.098	39.203	223.363	-50.5163

Table S463. Rh^{III}(DPES)(TFA^{eq})(TFAH^{eq})(CH$_3^{ax}$)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.36	-2399.4	-2399.11	205.44	17.828	45.098	36.852	118.84	-21.1911
498.15	-2399.36	-2399.4	-2399.18	205.44	45.643	47.648	38.382	190.1031	-21.1911

Table S464. [Rh^{III}(DPES)(TFAH^{eq})$_2$(CH$_3^{ax}$)]$^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.72	-2399.8	-2399.5	213.364	18.542	45.103	36.94	119.9917	-48.058
498.15	-2399.72	-2399.8	-2399.56	213.364	47.07	47.653	38.47	192.0476	-48.058

Table S465. Rh^{III}(DPES)(TFA^{ax})(TFAH^{eq})(CH$_3^{eq}$)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.35	-2399.38	-2399.1	205.742	18.614	45.098	37.009	121.3805	-19.9051
498.15	-2399.35	-2399.38	-2399.16	205.742	46.858	47.648	38.539	192.7364	-19.9051

Table S466. $[Rh^{III}(DPES)\ (TFA)_2(CH_3^{ax})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2398.86	-2398.95	-2398.68	198.082	18.187	45.093	36.922	123.3246	-56.7331
498.15	-2398.86	-2398.95	-2398.74	198.082	45.918	47.643	38.452	194.4033	-56.7331

Table S467. $[Rh^{III}(DPES)\ (TFA)_2(CH_3^{eq})]^-$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2398.85	-2398.94	-2398.67	197.65	18.933	45.093	36.895	125.0417	-54.2611
498.15	-2398.85	-2398.94	-2398.73	197.65	47.13	47.643	38.425	196.3009	-54.2611

Table S468. $[Rh^{III}(DPES)\ (TFAH)_2(CH_3^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.71	-2399.78	-2399.48	214.976	17.799	45.103	36.991	118.5177	-45.3553
498.15	-2399.71	-2399.78	-2399.54	214.976	45.794	47.653	38.521	190.2332	-45.3553

Table S469. $Rh^{IV}(DPES)\ (TFA)_2(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2398.68	-2398.73	-2398.46	198.634	18.023	45.093	36.815	121.6783	-27.3266
498.15	-2398.68	-2398.73	-2398.52	198.634	45.755	47.643	38.345	192.7638	-27.3266

Table S470. $Rh^{IV}(DPES)\ (TFA)_2(CH_3^{eq})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2398.68	-2398.72	-2398.45	198.266	18.743	45.093	36.765	123.1267	-23.6329
498.15	-2398.68	-2398.72	-2398.51	198.266	46.926	47.643	38.295	194.3505	-23.6329

Table S471. $[Rh^{IV}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.05	-2399.13	-2398.85	205.585	18.459	45.098	36.85	118.6338	-50.2486
498.15	-2399.05	-2399.13	-2398.91	205.585	46.786	47.648	38.38	190.2031	-50.2486

Table S472. $[Rh^{IV}(DPES)(TFA^{ax})(TFAH^{eq})(CH_3^{eq})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.05	-2399.12	-2398.84	205.983	18.702	45.098	36.97	121.7052	-48.3713
498.15	-2399.05	-2399.12	-2398.9	205.983	47.05	47.648	38.5	193.3311	-48.3713

Table S473. $Rh^{II}(DPES)(TFA)(TFAH)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.46	-2359.5	-2359.25	181.78	17.272	45.024	36.841	112.5706	-23.9696
498.15	-2359.46	-2359.5	-2359.31	181.78	43.519	47.574	38.372	178.8711	-23.9696

Table S474. $[Rh^{II}(DPES)(TFAH)_2]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2359.83	-2359.91	-2359.65	190.946	16.719	45.029	36.865	112.1836	-52.1424
498.15	-2359.83	-2359.91	-2359.71	190.946	42.808	47.579	38.395	179.0824	-52.1424

Table S475. $[Rh^{III}(DPES)(TFA^{eq})(CH_3{}^{ax}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.3	-2399.34	-2399.06	203.038	18.389	45.098	36.859	119.1417	-25.4315
498.15	-2399.3	-2399.34	-2399.12	203.038	46.612	47.648	38.389	190.4447	-25.4315

Table S476. $[Rh^{III}(DPES)(TFA^{eq})(CH_3{}^{eq}\text{-}H\text{-}TFA^{ax})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.31	-2399.34	-2399.06	203.171	18.302	45.098	36.88	118.6773	-23.1637
498.15	-2399.31	-2399.34	-2399.12	203.171	46.468	47.648	38.41	189.8312	-23.1637

Table S477. $[Rh^{III}(DPES)(TFA^{ax})(CH_3{}^{eq}\text{-}H\text{-}TFA^{eq})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2399.31	-2399.35	-2399.07	203.209	17.734	45.098	36.879	118.5425	-22.7471
498.15	-2399.31	-2399.35	-2399.13	203.209	45.516	47.648	38.41	189.731	-22.7471

Table S478. $[Rh^{III\text{-}I}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2925.59	-2925.67	-2925.37	221.848	22.459	45.606	38.403	159.4631	-49.7747
498.15	-2925.59	-2925.67	-2925.45	221.848	55.404	48.156	39.933	244.7754	-49.7747

Table S479. $[Rh^{III\text{-}I}(DPES)(TFAH^{eq})_2(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2926.06	-2926.1	-2925.79	230.919	22.814	45.61	38.355	156.6635	-24.1105
498.15	-2926.06	-2926.1	-2925.86	230.919	56.353	48.161	39.885	242.4563	-24.1105

Table S480. $[Rh^{III\text{-}II}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3926.71	-3926.67	-3926.39	209.864	22.872	45.84	38.585	161.169	25.7867
498.15	-3926.71	-3926.67	-3926.47	209.864	55.467	48.39	40.116	245.6777	25.7867

Table S481. $[Rh^{IV\text{-}II}(DPES)(TFA^{eq})(TFAH^{eq})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2925.44	-2925.48	-2925.18	222.093	23.203	45.606	38.274	154.4126	-24.7315
498.15	-2925.44	-2925.48	-2925.25	222.093	56.891	48.156	39.804	239.5864	-24.7315

Table S482. $[Rh^{IV\text{-}II}(DPES)(TFA)_2(CH_3{}^{ax}\text{-}TFA)]^{-\ddagger}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2924.95	-2925.04	-2924.75	214.572	23.069	45.602	38.297	159.9808	-56.928
498.15	-2924.95	-2925.04	-2924.83	214.572	56.324	48.152	39.827	245.093	-56.928

Table S483. $[Rh^{III}(DPES)(TFA^{eq})(CH_2TFA^{ax}\text{-}H\text{-}TFA^{eq})]^{\ddagger}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2924.84	-2924.88	-2924.58	216.306	22.077	45.602	37.83	145.5965	-25.861
498.15	-2924.84	-2924.88	-2924.66	216.306	55.106	48.152	39.36	229.0872	-25.861

Table S484. $[Rh^{III}(DPES)(TFA^{eq})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{ax})]^{\ddagger}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2924.85	-2924.89	-2924.59	216.19	22.082	45.602	37.826	145.6576	-24.9283
498.15	-2924.85	-2924.89	-2924.67	216.19	55.106	48.152	39.356	229.1305	-24.9283

Table S485. $[Rh^{III}(DPES)(TFA^{ax})(CH_2TFA^{eq}\text{-}H\text{-}TFA^{eq})]^{\ddagger}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2924.85	-2924.89	-2924.6	216.004	22.207	45.602	37.795	147.2488	-24.3633
498.15	-2924.85	-2924.89	-2924.67	216.004	55.291	48.152	39.325	230.8776	-24.3633

Rh(PN) complexes in TFAH

A P superscript (e.g. $TFAH^P$) refers to an equatorial ligand *trans* to the phosphine in the (PN) ligand, whereas an N superscript refers to an equatorial ligand *trans* to the nitrogen.

Table S486. $Rh^{I}(PN)(TFA^N)(TFAH^P)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2323.96	-2323.98	-2323.68	215.056	18.862	45.161	37.472	126.4198	-12.8434
498.15	-2323.96	-2323.98	-2323.75	215.056	47.841	47.711	39.002	199.5529	-12.8434

Table S487. $Rh^{I}(PN)(TFA^P)(TFAH^N)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2323.96	-2323.98	-2323.68	215.327	18.254	45.161	37.45	125.9227	-13.6169
498.15	-2323.96	-2323.98	-2323.75	215.327	46.814	47.711	38.98	199.0008	-13.6169

Table S488. $Rh^{III}(PN)(TFA)_3(TFAH^P)$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3376.29	-3376.32	-3375.98	252.569	27.264	46.086	38.697	189.3636	-17.6076
498.15	-3376.29	-3376.32	-3376.07	252.569	66.977	48.637	40.227	290.7592	-17.6076

Table S489. $Rh^{III}(PN)(TFA)_3(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3376.27	-3376.3	-3375.96	252.441	27.119	46.086	38.649	187.7088	-18.3907
498.15	-3376.27	-3376.3	-3376.05	252.441	66.854	48.637	40.179	289.1616	-18.3907

Table S490. $[Rh^{III}(PN)(TFA)_2(TFAH^{ax})(TFAH^{P})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3376.66	-3376.72	-3376.37	260.947	27.818	46.09	38.668	188.6248	-42.0565
498.15	-3376.66	-3376.72	-3376.46	260.947	68.229	48.64	40.198	290.7751	-42.0565

Table S491. $[Rh^{III}(PN)(TFA)_2(TFAH^{eq})_2]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3376.66	-3376.72	-3376.37	260.039	27.345	46.09	38.668	189.4938	-41.6731
498.15	-3376.66	-3376.72	-3376.46	260.039	67.305	48.64	40.198	291.4975	-41.6731

Table S492. $Rh^{III}(PN)(TFA)_2(TFAH^{P})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890.01	-2890.03	-2889.68	257.338	23.508	45.72	38.094	164.7525	-16.7236
498.15	-2890.01	-2890.03	-2889.76	257.338	59.294	48.27	39.624	257.1644	-16.7236

Table S493. $Rh^{III}(PN)(TFA)_2(TFAH^{N})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890	-2890.03	-2889.67	257.394	24.598	45.72	38.078	164.5911	-16.3098
498.15	-2890	-2890.03	-2889.75	257.394	61.196	48.27	39.608	257.0536	-16.3098

Table S494. $Rh^{III}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890.02	-2890.04	-2889.68	257.993	24.646	45.72	38.15	164.6443	-15.59
498.15	-2890.02	-2890.04	-2889.76	257.993	61.2	48.27	39.68	256.9903	-15.59

Table S495. $[Rh^{III}(PN)(TFA^{ax})(TFAH^{eq})_2(CH_3^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890.38	-2890.44	-2890.08	266.123	24.239	45.724	38.151	166.2012	-40.7805
498.15	-2890.38	-2890.44	-2890.16	266.123	60.651	48.274	39.681	259.184	-40.7805

Table S496. $[Rh^{III}(PN)(TFA^{N})(TFAH^{ax})(TFAH^{P})(CH_3^{ax})]^+$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890.39	-2890.45	-2890.09	266.214	24.873	45.724	38.175	167.3651	-39.5718
498.15	-2890.39	-2890.45	-2890.17	266.214	61.743	48.274	39.705	260.5076	-39.5718

Table S497. $[Rh^{III}(PN)(TFA^{P})(TFAH^{ax})(TFAH^{N})(CH_3{}^{ax})]^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890.38	-2890.45	-2890.08	265.987	24.896	45.724	38.186	167.719	-39.9357
498.15	-2890.38	-2890.45	-2890.16	265.987	61.738	48.274	39.716	260.7881	-39.9357

Table S498. $Rh^{III}(PN)(TFA^{ax})_2(TFAH^{P})(CH_3{}^{N})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2890	-2890.03	-2889.67	257.626	23.727	45.72	38.188	167.2565	-15.0333
498.15	-2890	-2890.03	-2889.76	257.626	59.527	48.27	39.718	259.7111	-15.0333

Table S499. $[Rh^{II}(PN)(TFA^{N})(TFAH^{P})]^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2323.7	-2323.77	-2323.47	216.336	18.975	45.161	37.458	127.9791	-43.2989
498.15	-2323.7	-2323.77	-2323.53	216.336	47.908	47.711	38.988	201.0003	-43.2989

Table S500. $[Rh^{II}(PN)(TFA^{P})(TFAH^{N})]^{+}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2323.69	-2323.76	-2323.47	215.963	18.368	45.161	37.416	127.5009	-43.4819
498.15	-2323.69	-2323.76	-2323.53	215.963	46.882	47.711	38.946	200.4633	-43.4819

Table S501. $[Rh^{III}(PN)(TFA)_2(CH_3{}^{ax}\text{-}H\text{-}TFA^{P})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2889.95	-2889.98	-2889.63	254.737	24.548	45.72	38.06	164.4589	-20.5611
498.15	-2889.95	-2889.98	-2889.71	254.737	61.109	48.27	39.59	256.8299	-20.5611

Table S502. $[Rh^{III}(PN)(TFA)_2(CH_3{}^{ax}\text{-}H\text{-}TFA^{N})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2889.95	-2889.98	-2889.63	254.982	24.463	45.72	38.119	164.4048	-19.0509
498.15	-2889.95	-2889.98	-2889.71	254.982	60.962	48.27	39.649	256.6142	-19.0509

Table S503. $[Rh^{III}(PN)(TFA^{ax})_2(CH_3{}^{N}\text{-}H\text{-}TFA^{P})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2889.96	-2889.99	-2889.64	254.866	23.916	45.72	38.119	163.6959	-18.1786
498.15	-2889.96	-2889.99	-2889.72	254.866	60.054	48.27	39.65	255.9972	-18.1786

Table S504. $[Rh^{III\text{-}I}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3416.26	-3416.33	-3415.96	274.596	29.8	46.139	39.363	205.6623	-43.3098
498.15	-3416.26	-3416.33	-3416.05	274.596	71.89	48.689	40.893	312.0751	-43.3098

Table S505. $[Rh^{III\text{-}I}(PN)(TFA^{N})(TFAH^{ax})(TFAH^{P})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3416.73	-3416.76	-3416.38	282.786	29.206	46.142	39.245	204.4237	-21.8349
498.15	-3416.73	-3416.76	-3416.48	282.786	71.148	48.692	40.775	311.4587	-21.8349

Table S506. $[Rh^{III\text{-}I}(PN)(TFA^{P})(TFAH^{ax})(TFAH^{N})(CH_3{}^{ax}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3416.72	-3416.75	-3416.37	281.805	28.537	46.142	39.183	203.899	-21.5866
498.15	-3416.72	-3416.75	-3416.47	281.805	69.946	48.692	40.713	310.5789	-21.5866

Table S507. $[Rh^{III\text{-}I}(PN)(TFA^{ax})_2(TFAH^{P})(CH_3{}^{N}\text{-}TFA)]^{-‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3416.25	-3416.31	-3415.94	273.826	29.219	46.139	39.252	204.5771	-40.7344
498.15	-3416.25	-3416.31	-3416.04	273.826	70.937	48.689	40.782	311.0566	-40.7344

Table S508. $[Rh^{III\text{-}I}(PN)(TFA^{ax})(TFAH^{ax})(TFAH^{P})(CH_3{}^{N}\text{-}TFA)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-3416.7	-3416.74	-3416.35	281.152	29.136	46.142	39.207	203.1598	-21.6444
498.15	-3416.7	-3416.74	-3416.45	281.152	70.957	48.692	40.737	309.8781	-21.6444

Table S509. $[Rh^{III\text{-}II}(PN)(TFA^{eq})_2(TFAH^{ax})(CH_3{}^{ax}\text{-}OVCl_3)]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-4417.28	-4417.31	-4416.96	262.338	28.505	46.336	39.414	207.1143	-15.8834
498.15	-4417.28	-4417.31	-4417.06	262.338	68.975	48.886	40.944	312.5233	-15.8834

Table S510. $[Rh^{I\text{-}III}(PN)(H^{N})(CH_3{}^{N})(TFA^{P})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.63	-1837.66	-1837.35	218.122	15.967	44.65	36.6	105.775	-16.3075
498.15	-1837.63	-1837.66	-1837.4	218.122	41.4	47.2	38.13	169.9018	-16.3075

Table S511. $[Rh^{I\text{-}III}(PN)(H^{N}\text{-}TFA)(CH_3{}^{N})(TFA^{P})]^{‡}$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2363.89	-2363.96	-2363.64	233.781	20.209	45.233	37.667	140.0427	-44.0561
498.15	-2363.89	-2363.96	-2363.71	233.781	51.078	47.783	39.197	218.9817	-44.0561

Table S512. $Rh^{I}(PN)(CH_3{}^{N})(TFAH^{P})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.63	-1837.65	-1837.34	219.768	15.502	44.65	36.562	106.6237	-10.2454
498.15	-1837.63	-1837.65	-1837.4	219.768	40.684	47.2	38.092	171.1186	-10.2454

Table S513. $Rh^{III}(PN)(H^{ax})(CH_3{}^{N})(\kappa^2\text{-}TFA^{ax,P})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.64	-1837.67	-1837.35	219.364	15.806	44.65	36.41	103.2181	-13.2747
498.15	-1837.64	-1837.67	-1837.41	219.364	41.42	47.2	37.94	167.7954	-13.2747

Table S514. $Rh^{III}(PN)(H^{ax})(CH_3{}^{N})(TFA^{P})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.63	-1837.66	-1837.35	218.493	15.603	44.65	36.594	107.1271	-16.9315
498.15	-1837.63	-1837.66	-1837.41	218.493	40.986	47.2	38.124	172.1354	-16.9315

Table S515. $Rh^{III}(PN)(H^{ax})(CH_3{}^{N})(TFA^{P})(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2364.42	-2364.44	-2364.1	243.966	20.669	45.237	37.588	138.5893	-12.7457
498.15	-2364.42	-2364.44	-2364.17	243.966	52.108	47.787	39.118	217.9354	-12.7457

Table S516. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.62	-1837.65	-1837.34	219.017	15.33	44.65	36.214	104.3888	-17.5962
498.15	-1837.62	-1837.65	-1837.4	219.017	40.57	47.2	37.744	169.0262	-17.5962

Table S517. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(\kappa^2\text{-}TFA^{ax,P})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.64	-1837.66	-1837.35	219.488	15.767	44.65	36.4	102.9066	-13.6915
498.15	-1837.64	-1837.66	-1837.41	219.488	41.34	47.2	37.93	167.3765	-13.6915

Table S518. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{P})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1837.63	-1837.66	-1837.35	219.249	15.999	44.65	36.616	105.8541	-16.998
498.15	-1837.63	-1837.66	-1837.4	219.249	41.619	47.2	38.146	170.4438	-16.998

Table S519. $Rh^{III}(PN)(H^{N})(CH_3{}^{ax})(TFA^{P})(TFAH^{ax})$

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-2364.43	-2364.45	-2364.11	244.118	20.561	45.237	37.514	137.5632	-12.8531
498.15	-2364.43	-2364.45	-2364.17	244.118	51.98	47.787	39.044	216.8569	-12.8531

Other

Table S520.

	H^+/TFAH	H^+/H_2O	e^-/TFAH	e^-/H_2O
Free energy	-260	-279.803	-127.063	-117.539

Table S521. CH_4 (g)

Temp	E_{gas}	G	ZPE	H_{tot}	S_{tot}
298.15	-40.4888	-40.4616	27.932	2.393	44.474
498.15	-40.4888	-40.4766	27.932	4.31	49.34

Table S522. TFAH (ℓ)

Temp	E_{gas}	G	ZPE	H_{tot}	S_{tot}	$\Delta G_{gas\rightarrow liquid}$
298.15	-526.753	-526.747	24.256	4.512	80.20577	-1.13846
498.15	-526.753	-526.768	24.256	9.917	93.91557	3.39033

Table S523. H_2O (ℓ)

Temp	E_{gas}	G	ZPE	H_{tot}	S_{tot}	$\Delta G_{gas\rightarrow liquid}$
298.15	-76.4183	-76.418	13.341	2.372	45.09052	-2.05333
498.15	-76.4183	-76.4247	13.341	4.005	49.27327	3.211233

Table S524. MeOH

Temp	E_{gas}	G	ZPE	H_{tot}	S_{tot}	Solv
298.15	-115.689	-115.665	32.007	2.702	57.021	-3.191 (aq)
498.15	-115.689	-115.68	32.007	5.263	63.506	0 (gas)

Table S525. $MeOH_2^+$ (aq)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-115.984	-116.114	-116.06	40.114	0.509	36.416	19.533	2.621529	-81.5237
498.15	-115.984	-116.114	-116.069	40.114	1.906	38.967	21.063	6.098291	-81.5237

Table S526. CH_3TFA (g)

Temp	E_{gas}	G	ZPE	H_{tot}	S_{tot}
298.15	-566.03	-565.997	41.695	5.582	88.84473
498.15	-566.03	-566.028	41.695	12.258	105.7598

Table S527. $OVCl_3$ (TFAH)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1527.33	-1527.34	-1527.34	4.978	2.32	41.332	26.729	14.077	-0.8268
498.15	-1527.33	-1527.34	-1527.36	4.978	5.264	43.882	28.259	21.583	-0.8268

Table S528. $OVCl_3$ (aq)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1527.33	-1527.33	-1527.34	4.978	2.32	41.332	26.729	14.077	1.11218
498.15	-1527.33	-1527.33	-1527.35	4.978	5.264	43.882	28.259	21.583	1.11218

Table S529. $MeOVCl_3$ (TFAH)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1567.21	-1567.21	-1567.18	28.766	4.057	41.582	29.793	27.567	-3.241
498.15	-1567.21	-1567.21	-1567.21	28.766	8.882	44.132	31.324	39.833	-3.241

Table S530. $MeOVCl_3$ (aq)

Temp	E_{gas}	E_{solv}	G	ZPE	H_{vib}	S_{trans}	S_{rot}	S_{vib}	Solv
298.15	-1567.21	-1567.21	-1567.18	28.766	4.057	41.582	29.793	27.567	-1.94225
498.15	-1567.21	-1567.21	-1567.2	28.766	8.882	44.132	31.324	39.833	-1.94225